

Gauge Theory of Dislocations in Solids and Melting as a Meissner-Higgs Effect.

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We develop a theory of interacting dislocation lines in analogy with the Ginzburg-Landau theory of superconductivity. The complex order parameter becomes a *disorder* parameter describing dislocation lines, the photon field turns into a gauge field of *phonons*. Above a certain temperature, the dislocation fields take nonzero expectation values which limit the phonon propagation to a finite penetration depth. In a cubic crystal, there are three would-be Nambu-Goldstone modes associated with the phase oscillations of the fields of the basic dislocation lines for the three space axes. Their transverse projections are «eaten up» by the gauge field. Their longitudinal part survives, representing the sound waves in the molten phase (*hot sound* as the disorder analogue to zero sound = «cool sound»).

In recent years, local gauge invariance has become a universal building principle of theories of fundamental interactions⁽¹⁾. As gauge fields are coupled to complex scalar fields $\psi(\mathbf{x})$ they give rise to a phenomenon called Meissner-Higgs effect: If the scalar fields form a condensate with $\langle\psi(\mathbf{x})\rangle \equiv \psi^0 \neq 0$, the symmetry $\psi(\mathbf{x}) \rightarrow \exp[-i\alpha]\psi(\mathbf{x})$ is spontaneously broken and the phase oscillations $\psi^0(\mathbf{x}) = \exp[-i\gamma(\mathbf{x})]\psi^0$ form Nambu-Goldstone bosons (NGBs). The gauge field, however, absorbs these, becomes massive and loses its long-range propagation. The Ginzburg-Landau free energy of a type-II superconductor provides the best-known example for this mechanism:

$$(1) \quad f(\mathbf{x}) = |(\nabla_i - ieA_i)\psi(\mathbf{x})|^2 + m^2|\psi(\mathbf{x})|^2 + \frac{g}{2}|\psi(\mathbf{x})|^4 + \frac{1}{4}(\partial_i A_j(\mathbf{x}) - \partial_j A_i(\mathbf{x}))^2.$$

At the mean-field level, a phase transition occurs if $m^2 \sim (T/T_c - 1)$ becomes negative ($T < T_c$) in which case the field $\psi(\mathbf{x})$ of Cooper pairs takes a nonvanishing expectation value

$$(2) \quad \langle\psi(\mathbf{x})\rangle \equiv \psi^0(\mathbf{x}) = \exp[-i\gamma(\mathbf{x})] \sqrt{-\frac{m^2}{g}},$$

⁽¹⁾ C. ITZYKSON and J.-B. ZUBER: *Quantum Field Theory* (New York, N.Y., 1980).

signalizing the formation of a condensate of Cooper pairs. The phase $\gamma(\mathbf{x})$ of the $\psi^0(\mathbf{x})$ field can be absorbed into A_i by a gauge transformation and disappears (« $\gamma \equiv 0$ gauge »). The photon field receives a mass term

$$(3) \quad e^2 |\psi^0|^2 A_i^2 = \frac{1}{2} e^2 |m^2| A_i^2,$$

which limits the penetration of the magnetic field in the superconductor to a length scale $l \sim 1/e|m|$. The phenomenon is called Meissner effect, while the absorption of the NGB was first elucidated field-theoretically by HIGGS⁽²⁾.

The Ginzburg-Landau free energy has another property, which, in superconductors, is quite unimportant, but which will be essential in our considerations⁽³⁾. If the fluctuations of the photon field are taken into account, the partition function becomes

$$(4) \quad Z = \int \mathcal{D}A \exp \left[-\frac{1}{T} \int d^3x f(\mathbf{x}) \right] = \\ = \exp \left[-\frac{1}{T} \int d^3x \left\{ f^{A=0} + T \int \frac{d^3k}{(2\pi)^3} \log(k^2 + e^2 |\psi|^2) \right\} \right],$$

where $\psi(\mathbf{x})$ has been made real by a pure gauge transformation and *assumed constant*. The fluctuation integral over d^3k can be performed and gives, up to diverging but trivial renormalizations of mass and interaction strength, $-(T/6\pi)e^3|\psi|^3$ such that the free energy for a constant $|\psi|$ -field becomes

$$(5) \quad f = m^2 |\psi|^2 + \frac{g}{2} |\psi|^4 - \frac{T}{6\pi} e^3 |\psi|^3.$$

Here we observe that the fluctuation correction has the consequence that, instead of the original second-order transition at $m^2 = 0$, there is now a first-order transition at a *precocious* value⁽³⁾

$$(6) \quad m_{\text{prec}}^2 = \frac{1}{2} \frac{T^2}{(6\pi)^2} e^6/g > 0.$$

In order to believe this result, we have to make sure that the assumption $\psi = \text{const}$ is self-consistent. For this we compare m_{prec}^2 with the interval of large fluctuations of the ψ -field estimated by the Landau criterion $|m^2| \leq m_{\text{L}}^2 = 4T^2 g^2$ which specifies the point where condensation energy $m^4/2g$ times the coherence volume $(m^2)^{-3/2}$ equals the thermal energy T . If we denote $K \equiv \sqrt{g/e^2}$, we see $m_{\text{L}}^2 = 8(6\pi)^2 K^6 m_{\text{prec}}^2$. Now, type-II superconductors have $K > 1/\sqrt{2}$ such that fluctuations are expected to invalidate the argument. In fact, the transition is always observed to be of second order. If, however, a superconductor is deeply of type I, $K \ll 1/\sqrt{2}$ and m_{prec}^2 lies outside the Landau interval, fluctuations are small and the assumption of $\psi = \text{const}$ is, indeed, self-consistent, making the transition of first order (*).

It is the purpose of this note to point out that the process of melting in solids can be understood by a completely analogous field theory: Cooper pairs need only be replaced by dislocations, photons by phonons. The condensation of dislocations, *i.e.*

(²) P. W. HIGGS: *Phys. Rev.*, **145**, 1156 (1966); T. W. B. KIBBLE: *Phys. Rev.*, **155**, 1544 (1967).

(³) B. H. HALPERIN, T. C. LUBENSKY and S. K. MA: *Phys. Rev. Lett.*, **32**, 292 (1974).

(*) The transition point between first and second order is $K \approx 1.1/\sqrt{2}$ as shown by H. KLEINERT: *Lett. Nuovo Cimento* (in press).

their proliferations, gives the phonons a finite penetration depth. The sound waves in the molten state are carried by a « left-over » NGB which the gauge field is incapable of absorbing.

The value of K is so small to m_{pre}^2 is large and the transition is of first order. In more physical terms, the elastic forces play an important role in making the defects proliferate at much lower temperature than they would on entropy grounds alone, thereby causing a *strongly precocious* melting.

There is no problem in constructing a gauge theory of the elasticity energy itself. It depends on the symmetric stress tensor σ_{ij} in the well-known way⁽⁴⁾:

$$(7) \quad f_{\text{ph}} = \frac{1}{4\mu} \left(\sigma_{ij}^2 - \frac{\nu}{1+\nu} \sigma_{ii}^2 \right)$$

with μ, ν being modulus of rigidity and Poisson number, respectively. In the absence of local body forces, σ_{ij} is divergenceless and can be written as a double curl of a symmetric tensor A_{ln} which we shall shortly call the phonon field:

$$(8) \quad \sigma_{ij} = \varepsilon_{ikl} \varepsilon_{jmn} \nabla_k \nabla_m A_{ln}.$$

By construction, σ_{ij} and f_{ph} are invariant under local gauge transformations

$$(9) \quad A_{ln}(\mathbf{x}) \rightarrow A_{ln}(\mathbf{x}) - \nabla_l A_n(\mathbf{x}) - \nabla_n A_l(\mathbf{x}),$$

where $A_l(\mathbf{x})$ is an arbitrary vector field.

Consider now dislocation lines. For simplicity we shall assume that a single line can move through the crystal in a complete random way with all configurations having equal probability.

For a single open random chain of length $s' - s$ in a simple cubic lattice, the probability to run from \mathbf{x} to \mathbf{x}' is⁽⁵⁾

$$(10) \quad \begin{aligned} P(\mathbf{x}' - \mathbf{x}, s' - s) &= \theta(s' - s) \int \mathcal{D}x \exp \left[-\frac{M}{2} \int_0^{s'-s} dt \dot{\mathbf{x}}^2(t) \right] = \\ &= \theta(s' - s) \sqrt{2\pi(s' - s)/M}^3 \exp \left[-\frac{M}{2} \frac{(\mathbf{x}' - \mathbf{x})^2}{s' - s} \right] = \\ &= \theta(s' - s) \int \frac{d^3k}{(2\pi)^3} \exp \left[i\mathbf{k}(\mathbf{x}' - \mathbf{x}) - \frac{k^2}{2M} (s' - s) \right], \end{aligned}$$

where the mass M is given by the lattice constant l as $M = 3/l$. In a grand-canonical ensemble of chains, the lengths $s' - s$ are arbitrary. A single chain can appear in $\mathcal{G}^{(s'-s)/l} \equiv \exp[w(s' - s)]$ possible configurations, such that \mathbf{x} and \mathbf{x}' can be connected in $\exp[-w(s' - s)]P(\mathbf{x}' - \mathbf{x}, s' - s)$ ways. The thermal creation of these chains is governed by a Boltzmann factor $\exp[-(\varepsilon_{\text{core}}/T)(s' - s)]$. Thus we obtain for the prob-

⁽⁴⁾ L. D. LANDAU and E. M. LIFSHITZ: *Theory of Elasticity* (New York, N. Y., 1959); E. KRÖNER: *Kontinuumstheorie der Versetzungen und Eigenspannungen*, *Ergeb. Angew. Math.*, **5**, 1958 and Proceedings Summer School on *The Physics of Defects*, Les Houches, France (1980).

⁽⁵⁾ H. YAMAKAWA: *Modern Theory of Polymer Solutions* (New York, N. Y., 1971).

ability of finding a chain of any length through \mathbf{x} and \mathbf{x}'

$$(11) \quad P(\mathbf{x}' - \mathbf{x}) = \int_{-\infty}^{\infty} d(s' - s) \exp \left[-\frac{\varepsilon(s' - s)}{T} \right] P(\mathbf{x}' - \mathbf{x}, s' - s) = \\ = \int \frac{d^3k}{(2\pi)^3} \frac{2M}{k^2 + (\varepsilon/T) 2M} \exp [ik(\mathbf{x}' - \mathbf{x})]$$

with $\varepsilon = m^2 - wT$. For many chains, the joint probability is given by the symmetrical product

$$(12) \quad \frac{1}{N!} \sum_{p(i)} P(\mathbf{x}_1 - \mathbf{x}_{p(1)}) P(\mathbf{x}_2 - \mathbf{x}_{p(2)}) \dots, P(\mathbf{x}_N - \mathbf{x}_{p(N)}),$$

This can also be obtained from the generating functional of a fluctuating field theory

$$(13) \quad Z_1[\eta^+, \eta] = \int \mathcal{D}\varphi \mathcal{D}\varphi^+ \exp \left[- \int d^3x \left(\frac{1}{2M} |\nabla\varphi|^2 + \frac{\varepsilon}{T} |\varphi|^2 + \eta^+ \varphi + \varphi^+ \eta \right) \right]$$

by partial differentiation with respect to the sources η^+ and η . For $\eta = \eta^+ = 0$, Z represents the partition function of a grand canonical ensemble of closed dislocation lines. Integrating out of the φ -fields gives

$$(14) \quad Z_1[0, 0] = \exp \left[- \text{tr} \log \left(-\frac{1}{2M} \nabla^2 + \frac{\varepsilon}{T} \right) \right] = \sum_N \frac{1}{N!} Z_1^N.$$

But Z_1 can be rewritten as

$$(15) \quad Z_1 = - \text{tr} \log \left(-\frac{1}{2M} \nabla^2 + \frac{\varepsilon}{T} \right) = \frac{1}{T} \int_0^{\infty} d\varepsilon \int d^3x P(\mathbf{x}, \mathbf{x}) = \\ = \frac{1}{T} \int_0^{\infty} d\varepsilon \int d^3x \int_{-\infty}^{\infty} d(s' - s) \exp \left[-\frac{\varepsilon}{T} (s' - s) \right] P(\mathbf{x}, \mathbf{x}, s' - s) = \\ = \int_{-\infty}^{\infty} d(s' - s)/l \exp \left[-\frac{m^2}{T} (s' - s) \right] \left[\int d^3x \frac{1}{(s' - s)/l} \exp [w(s' - s)] P(\mathbf{x}, \mathbf{x}, s' - s) \right]$$

and the expression in brackets is recognized as the total number of possible closed-chain configurations in the crystal, which proves our statement.

This formalism can be used for dislocation lines if we introduce a field $\varphi_{\mathbf{b}}(\mathbf{x})$ for every Burgers vector \mathbf{b} . Actually, just as nuclei can be composed of protons and neutrons with two-body forces, we shall assume, by analogy, that all higher dislocation lines can be generated from the three fundamental ones in which a single atomic layer is missing in one lattice direction. Thus we introduce the steric interaction

$$(16) \quad F_{\text{int}} = \int d^3x d^3x' \varphi_{\mathbf{b}}^{\dagger}(\mathbf{x}) \varphi_{\mathbf{b}}(\mathbf{x}) \varphi_{\mathbf{b}'}^{\dagger}(\mathbf{x}') \varphi_{\mathbf{b}'}(\mathbf{x}') V_{\mathbf{b}\mathbf{b}'}(\mathbf{x} - \mathbf{x}'),$$

where the range of V is a few lattice spacings. For the purpose of studying the phase transition of melting, we shall be content with the quasi-local approximation

$$V_{bb'} \sim \frac{1}{4M^2} g_{bb'} \delta(\mathbf{x} - \mathbf{x}').$$

To this grand canonical ensemble of dislocation lines with steric interactions, we now couple the stress field. We shall do this in a gauge-invariant fashion via the minimal substitution (analogous to $\nabla_l \rightarrow \nabla_l - ieA_l$ in electromagnetism) (1):

$$(17) \quad \nabla_l \rightarrow \nabla_l - i \frac{1}{T} b_i' \varepsilon_{ijk} \nabla_j A_{kl},$$

where b_i is the fixed Burgers vector for each dislocation line. In this way, a gauge transformation (9) can be compensated by a local phase change

$$(18) \quad \psi(\mathbf{x}, s) \rightarrow \exp[-i\alpha(\mathbf{x})] \psi(\mathbf{x}, s)$$

with

$$(19) \quad \alpha(\mathbf{x}) = \frac{1}{T} \mathbf{b} \cdot (\nabla \times \Lambda).$$

In this way we arrive at an energy density

$$(20) \quad f(\mathbf{x}) = \sum_{\mathbf{b}} \left[\left| \left(\nabla_l - i \frac{1}{T} b_i \varepsilon_{ijk} \nabla_j A_{kl} \right) \varphi_{\mathbf{b}} \right|^2 + 2M(m^2 - wT) |\varphi_{\mathbf{b}}|^2 \right] + \\ + \frac{1}{2} \sum_{\mathbf{b}, \mathbf{b}'} g_{\mathbf{b}\mathbf{b}'} |\varphi_{\mathbf{b}}|^2 |\varphi_{\mathbf{b}'}|^2 + \frac{1}{4\mu} \left(\sigma_{ij}^2 - \frac{\nu}{1+\nu} \sigma_{ii}^2 \right)$$

in close analogy with (1).

Let us first convince ourselves that with this gauge theory we are able to reproduce correctly the elastic forces between dislocations. For this we have to calculate the propagator of the A_{ln} field by writing

$$(21) \quad \int d^3x f_{\text{ph}}(\mathbf{x}) = \sum_{\mathbf{k}} A_{ln}(\mathbf{k}) D_{ln,l'n'}(\mathbf{k}) A_{l'n'}(\mathbf{k})$$

and invert the matrix

$$(22) \quad D_{ln,l'n'}(\mathbf{k}) = \mathbf{k}^4 \left[(\delta_{ll'} - \hat{k}_l \hat{k}_{l'}) (\delta_{nn'} - \hat{k}_n \hat{k}_{n'}) - \frac{\nu}{1+\nu} (\delta_{ln} - \hat{k}_l \hat{k}_n) (\delta_{l'n'} - \hat{k}_{l'} \hat{k}_{n'}) \right]$$

in the subspace of physical components of $A_{ln}(\mathbf{k})$ which are orthogonal to the three gauge degrees of freedom (9). In order to do so, we decompose $A_{ln}(\mathbf{k})$ into spin- s helicity- λ components

$$A_{ln}(\mathbf{k}) = \sum_{\substack{s=0,2 \\ \lambda=-s, \dots, s}} \varepsilon_{ln}^{(s,\lambda)}(\mathbf{k}) A^{(s,\lambda)}(\mathbf{k}).$$

Moreover, instead of $\varepsilon_{ln}^{(0,0)}$, $\varepsilon_{ln}^{(2,0)}$, we shall prefer to use certain combinations of these longitudinal components:

$$\varepsilon^L = \frac{1}{\sqrt{3}} (\sqrt{2}\varepsilon^{(0,0)} - \varepsilon^{(2,0)}), \quad \varepsilon^{L'} = \frac{1}{\sqrt{3}} (\varepsilon^{(0,0)} + \sqrt{2}\varepsilon^{(2,0)}).$$

If we then define the projections into the channels $(s, \lambda), L, L'$ by $P_{ln,l'n'}(\mathbf{k}) \equiv \varepsilon_{ln}(\hat{k})\varepsilon_{l'n'}(\hat{k})^*$ such that $P^{(2,2)} + P^{(2,-2)} + P^{(2,1)} + P^{(2,-1)} + P^L + P^{L'} = 1|_{\text{sym}}$, we find that the free energy (21) takes the form

$$(23) \quad \int d^3x f_{\text{ph}} = \sum_{\mathbf{k}} \frac{1}{4\mu} \mathbf{k}^4 A(\mathbf{k}) \left[P^{(2,2)} + P^{(2,-2)} + \frac{1-\nu}{1+\nu} P^L \right] A(\mathbf{k}),$$

thereby exhibiting the three-dimensional physical subspace of $A_{ln}(\mathbf{k})$'s. Within it, we may immediately invert the matrix in brackets and find the propagator

$$(24) \quad \langle A_{ln}(\mathbf{k}) A_{l'n'}(\mathbf{k}) \rangle = \frac{2\mu T}{\mathbf{k}^4} \left[P^{(2,2)} + P^{(2,-2)} + \frac{1+\nu}{1-\nu} P^L \right]_{ln,l'n'} = \\ = \frac{2\mu T}{\mathbf{k}^4} \left[(\delta_{ll'} - \hat{k}_l \hat{k}_{l'}) (\delta_{nn'} - \hat{k}_n \hat{k}_{n'}) + \frac{\nu}{1-\nu} (\delta_{ln} - \hat{k}_l \hat{k}_n) (\delta_{l'n'} - \hat{k}_{l'} \hat{k}_{n'}) \right].$$

Consider now two dislocation lines running, say, along the paths $\mathbf{x}(s), \mathbf{x}'(s)$. For a single line, the second quantized coupling

$$(25) \quad \frac{l}{6_i} b_i \int d^3x \int ds \psi^+(\mathbf{x}, s) \vec{\nabla}_l \psi(\mathbf{x}, s) \varepsilon_{ijk} \nabla_j A_{kl}(\mathbf{x})$$

becomes

$$(26) \quad b_i \int d^3x \int ds \frac{dx_l}{ds} \delta^{(3)}(\mathbf{x} - \mathbf{x}(s)) \varepsilon_{ijk} \nabla_j A_{kl}(\mathbf{x}).$$

Thus, using the propagator (24), the interaction energy between two lines is obtained as

$$(27) \quad E = \frac{1}{T} b_i b'_i \iint dx_l dx'_l \varepsilon_{ikl} \varepsilon_{i'k'l'} \langle \nabla_k A_{ln} \nabla_{k'} A_{l'n} \rangle = \\ = \frac{\mu}{4\pi} \iint \left[(\mathbf{b} \cdot d\mathbf{x})(\mathbf{b}' \cdot d\mathbf{x}')/R - (\mathbf{b} \times \mathbf{b}') \cdot (d\mathbf{x} \times d\mathbf{x}')/R + \frac{1}{1-\nu} (\mathbf{b} \times d\mathbf{x})_k (\mathbf{b}' \times d\mathbf{x}')_l \nabla_k \nabla_l R \right].$$

This is precisely the formula derived by BLIN⁽⁶⁾ many years ago on the basis of the classical elasticity theory.

Suppose now the temperature is moved up so high that $m^2 - wT$ becomes negative. Then ψ acquires a nonvanishing expectation value $\langle \psi \rangle \equiv \psi^0$ as a signal for a proliferation of dislocations. In cubic crystals in which the basic Burgers vectors point along $\mathbf{x}, \mathbf{y}, \mathbf{z}$, there is a dislocation field ψ_1, ψ_2, ψ_3 associated with each of these. For

(6) J. BLIN: *Acta Met.*, **3**, 199 (1955).

symmetry reasons, we expect the ψ interactions to stabilize, above the melting point, three equal-size nonzero expectation values $\psi_i^0(\mathbf{x}) = \exp[-i\gamma_i(\mathbf{x})]\psi^0$ ($i = 1, 2, 3$). Then the A_{kl}^2 term in (20) has to be summed over the three \mathbf{b} directions giving $|\psi^0|^2 b^2 k^2$ times

$$[|A_{ln}|^2 - \hat{k}_l \hat{k}_{l'} A_{ln}^\dagger A_{l'n}] = A^\dagger [P^{(2,2)} + P^{(2,-2)} + P^L + \frac{1}{2}(P^{(2,1)} + P^{(2,-1)})] A.$$

Thus we find, just as in the superconductor, that the gauge field ceases to propagate ($P^{(2,1)} + P^{(2,-1)}$ projects onto an irrelevant gauge degree of freedom).

Where is the sound wave known to exist in liquids? It is carried by the longitudinal projection of the phase oscillations of the fields $\psi_i^0(x)$, just as zero sound is in superfluid ^3He . In order to see this, we observe that in the absence of phonons there would be three NGBs associated with the phases $\gamma_1, \gamma_2, \gamma_3$. The Higgs effect, however, removes all those from the excitation spectrum which can be absorbed in a gauge transformation. If we express the derivative piece in (20) in terms of $\gamma_i(\mathbf{x})$, we find

$$|\psi^0|^2 \sum_i \left(\nabla_i \gamma_i(x) + \frac{1}{T} |\mathbf{b}| \varepsilon_{ijk} \nabla_j A_{kl}(x) \right)^2$$

and realize that, under the gauge transformations $\gamma_i \rightarrow \gamma_i + |\mathbf{b}|(1/T)(\nabla \times A)_i$. Therefore, the transverse projection $\gamma_i^\dagger \equiv (\delta_{ij} - \hat{k}_i \hat{k}_j) \gamma_j$ can be absorbed into the gauge field. The longitudinal part $\gamma_i^l \equiv \hat{k}_i \hat{k}_j \gamma_j$, however, survives as a long-range physical excitation which may be associated with the sound wave in the molten state of matter.

Because of its analogy to zero sound in ^3He (= « cool sound »), we propose to call the longitudinal NGB *hot sound*. Cool sound is carried by the phase of an order parameter, hot sound by that of a disorder parameter.

From the discussion of ref. (7) we know that, actually, there will remain directional order even if all basic dislocation lines proliferate. The result of the present melting process will be a liquid crystal rather than a liquid. In order to arrive at a proper liquid state, defects destroying orientational order must be included (disclinations). This will be done in a future work along the lines presented here.

In two dimensions, there exists some understanding of these successive steps in the melting process (7). We are convinced that our field theory, when properly extended to include disclinations, will clarify the physics in the three-dimensional situation (8).

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(7) B. I. HALPERIN and D. R. NELSON: *Phys. Rev. Lett.*, **41**, 121 (1978); D. R. NELSON and J. TONER: *Phys. Rev. B*, **24**, 363 (1981) and references therein.

(8) For further development see H. KLEINERT: *Phys. Lett. A*, **90**, 259 (1982); *Phys. Lett. B*, **113**, 395 (1982); *J. Phys. (Paris)* (in press) and *Lett. Nuovo Cimento*, **34**, 225 (1982), also in the context of the smectic nematic transition, magnetic superconductors, and pion condensates.