Interaction Energy between Defects in Higher-Gradient Elasticity.

H. KLEINERT (*)
Institüt für Theoretische Physik - 1 Berlin 33, Arnimalle 14

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Summary. – In linear elasticity, the interaction energy between defects depends only on the total defect tensor

$$\eta_{ij}(\boldsymbol{x}) = \theta_{ij}(\boldsymbol{x}) - \tfrac{1}{2}\big(\varepsilon_{ikl}\partial_k\alpha_{jl}(\boldsymbol{x}) + (ij)\big) + \tfrac{1}{2}\varepsilon_{ijk}\partial_l\alpha_{lk}(\boldsymbol{x})$$

and not on the particular composition in terms of the 6 + 6 components of the dislocation and disclination densities $\alpha_{ij}(\boldsymbol{x})$ and $\theta_{ij}(\boldsymbol{x})$, respectively. In momentum space, this energy is

$$E_{\text{def}} = \mu\sum_{\boldsymbol{q}}\frac{1}{\boldsymbol{q}^4}\left(|\eta_{ij}(\boldsymbol{q})^2 + \frac{\nu}{1-\nu}\,|\eta_{ll}(\boldsymbol{q})|^2\right).$$

We show that higher gradients in the elastic energy give the additional defect energy

$$\Delta E_{\text{def}} = \mu l'^2\sum_{\boldsymbol{q}}\frac{1}{\boldsymbol{q}^2(1+l'^2\boldsymbol{q}^2)}\,\frac{1-2\nu}{1-\nu}\,|\eta_{ll}|^2 + $$
$$+ 2\mu l^2\sum_{\boldsymbol{q}}\left\{\left(\frac{1+\varepsilon}{\boldsymbol{q}^2}\,|\theta_{ij}|^2 + \frac{1}{1+l^2\boldsymbol{q}^2}\,\frac{1}{\boldsymbol{q}^2}\,|\partial_j\alpha_{ij}{}^{\mathrm{T}}|^2 + \frac{1+\varepsilon}{4\boldsymbol{q}^4}\,|\boldsymbol{\partial}^2\alpha_{ll}{}^{\mathrm{T}} + \varepsilon_{ilk}\partial_i\theta_{lk}|^2\right) - \right.$$
$$\left. - \varepsilon\frac{1+\varepsilon l^2\boldsymbol{q}^2}{1+l^2\boldsymbol{q}^2}\,\frac{1}{\boldsymbol{q}^4}\,|\partial_j\theta_{ij}|^2 - \frac{\varepsilon}{\boldsymbol{q}^2}\,|\theta_{ll}|^2 + \frac{\varepsilon}{1+l^2\boldsymbol{q}^2}\,\frac{1}{\boldsymbol{q}^2}\,(\partial_j\alpha_{ij}{}^{\mathrm{T}*}\,\varepsilon_{ipq}\theta_{pq} + \text{c.c.})\right\},$$

where $\alpha_{ij}{}^{\mathrm{T}} \equiv (\delta_{jk} - \partial_j\partial_k/\boldsymbol{\partial}^2)\alpha_{ik}$. This removes the degeneracy for all 6 + 6 components of α_{ij} and θ_{ij}. The elastic constants are defined in the text.

Within linear elasticity, a large variety of defect distributions is energetically indistinguishable. The only quantity that determines the physically observable stress is

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the total defect density [1]

(1) $$\eta_{ij}(\boldsymbol{x}) = \varepsilon_{ikl}\varepsilon_{jmn}\partial_k\partial_m u_{ln}(\boldsymbol{x}) ,$$

(where $u_{ln}(\boldsymbol{x}) \equiv (\partial_l u_k(\boldsymbol{x}) + \partial_k u_l(\boldsymbol{x}))/2$). This tensor is symmetric and conserved ($\partial_i\eta_{ij}(\boldsymbol{x}) = 0$) and contains, therefore, only three independent components per sites $\boldsymbol{x}$. The set of *all* linelike defects, however, is classified by the the full symmetry group of the solid which, in the continuum approximation, becomes the Euclidean group such that there are dislocations with Burgers vector $\boldsymbol{b}$ (for translations) and disclinations with Frank vector $\boldsymbol{\Omega}$ (for rotations). Their distributions are described by a dislocation density

(2) $$\alpha_{ij}(\boldsymbol{x}) \equiv \varepsilon_{ikl}\partial_k\partial_l u_j(\boldsymbol{x})$$

and a disclination density

(3) $$\theta_{ij}(\boldsymbol{x}) \equiv \varepsilon_{ikl}\partial_k\partial_l\omega_j(\boldsymbol{x}) ,$$

(where $\omega_i(\boldsymbol{x}) \equiv \frac{1}{2}\varepsilon_{ijk}\partial_j u_k(\boldsymbol{x})$). The possibility of these being nonzero stems from the multivaluedness of the displacement and rotation fields $u_i(\boldsymbol{x})$ and $\omega_i(\boldsymbol{x})$ [2]. The densities satisfy the conservation laws

(4) $$\partial_i\theta_{ij}(\boldsymbol{x}) = 0 , \qquad \partial_i\alpha_{ij}(\boldsymbol{x}) = -\varepsilon_{jkl}\theta_{kl}(\boldsymbol{x}) .$$

Hence each of them possesses 6 independent matrix elements per site $\boldsymbol{x}$. It is easy to work out [1] that η_{ij} contains α_{ij} and θ_{ij} in the following combination:

(5) $$\eta_{ij}(\boldsymbol{x}) = \theta_{ij}(\boldsymbol{x}) - \tfrac{1}{2}\left(\varepsilon_{jkl}\partial_k\alpha_{jl}(\boldsymbol{x}) + (ij)\right) + \tfrac{1}{2}\varepsilon_{ijk}\partial_l\alpha_{lk}(\boldsymbol{x}) .$$

In this relation, the antisymmetric parts of θ_{ij} cancel with the divergence of α_{ij}. If $\alpha_{ij}{}^{\mathrm{T}}$ denotes the divergenceless part of α_{ij} and θ^{s}_{ij} the symmetric part of θ_{ij}, we can also write

(6) $$\eta_{ij}(\boldsymbol{x}) = \theta^{\mathrm{s}}_{ij}(\boldsymbol{x}) - \tfrac{1}{2}\left(\varepsilon_{ikl}\partial_k\alpha_{jl}{}^{\mathrm{T}}(\boldsymbol{x}) + (ij)\right) .$$

Thus, the linear elastic energy of arbitrary defect distributions depends only on a specific combination of the 12 independent components of θ_{ij} and $\alpha_{ij}{}^{\mathrm{T}}$. It is independent of the three antisymmetric components, θ^{a}_{ij}, and those of three components of α_{ij} which do not survive the curl operation in (6).

This 9-fold degeneracy of η_{ij} in terms of α_{ij} and θ_{ij} can be formulated as an invariance under a certain class of gauge transformations. Such a formulation is useful for understanding the structural interdependence among the different types of defects.

When developing statistical models of defect ensembles [3-5] it is important to remove this degeneracy (« gauge fixing ») [6]. Otherwise, the partition function acquires

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(1) E. KRÖNER: in *The Physics of Defect*, edited by R. BALIAN, G. 'T HOOFT, A. JAFFE, H. LEHMANN, P. K. MITTER, I. M. SINGER and R. STORA (Amsterdam, 1981).
(2) H. KLEINERT: *Lectures presented at the 1982 Cargèse Summer School on Gauge Theories*, edited by G. 'T HOOFT, A. JAFFE, H. LAHMANN, P. K. MITTER and J. M. SINGER (New York, N. Y.).
(3) H. KLEINERT: *Phys. Lett. A*, **89**, 294 (1982); **91**, 295 (1982); **93**, 82 (1982); *Lett. Nuovo Cimento*, **37**, 425 (1983).
(4) H. KLEINERT: *Phys. Lett. A*, **95**, 493 (1983).
(5) H. KLEINERT: *Phys. Lett. A*, **97**, 51 (1983).
(6) H. KLEINERT: *Gauge Theory of Stresses and Defects* (New York, N.Y., 1984), to be published.

infinite overall factors. This is usually done by attributing, to the defects, certain *ad hoc* core energies (sometimes derived from bond counting). Such a procedure can, however, be quite dangerous, since it might destroy the interdependence between dislocations and disclinations (7).

It is the purpose of this note to remove the degeneracy in a systematic way, namely by calculating the defect energies in a theory of elasticity which contains the next higher gradients of the displacement field $u_i(\boldsymbol{x})$. This produces definite modifications of the near-zone elastic fields and gives specifies core energies to each type of defect line.

The starting point is the higher-gradient elastic energy (8) in the presence of plastic distortions and rotations (6)

$$(7)\qquad E_{\text{el}} = \int d^3x \Big\{ \mu(u_{ij} - u_{ij}{}^P)^2 + \frac{\lambda}{2}(u_{ii} - u_{ii}{}^P)^2 + \\ + \tfrac{1}{2}(2\mu + \lambda)\, l'^2 (\partial_i u_{ll} - \partial_i u_{ll}{}^P)^2 + 2\mu l^2 [(\partial_i \omega_j - \tfrac{1}{2}\partial_i \varepsilon_{jkl}\partial_k u_l{}^P - \partial_i \omega_j{}^P)^2 + \\ + \varepsilon(\partial_i \omega_j - \tfrac{1}{2}\partial_i \varepsilon_{jkl}\partial_k u_l{}^P - \partial_i \omega_j{}^P)(\partial_j \omega_i - \tfrac{1}{2}\partial_j \varepsilon_{ikl}\partial_k u_l{}^P - \partial_j \omega_i{}^P)] \Big\} .$$

This energy is invariant under defect gauge transformations

$$(8)\qquad \begin{cases} \partial_i u_j{}^P(\boldsymbol{x}) \to \partial_i u_j{}^P(\boldsymbol{x}) + \partial_i N_i(\boldsymbol{x}) - \varepsilon_{ijq} M_q(\boldsymbol{x}) , \\ \partial_i \omega_j{}^P(\boldsymbol{x}) \to \partial_i \omega_j{}^P(\boldsymbol{x}) + \partial_i M_j(\boldsymbol{x}) , \\ u_i(\boldsymbol{x}) \to u_i(\boldsymbol{x}) + N_i(\boldsymbol{x}) , \\ \omega_i(\boldsymbol{x}) \to \omega_i(\boldsymbol{x}) + \tfrac{1}{2}\varepsilon_{ikl}\partial_k N_l(\boldsymbol{x}) . \end{cases}$$

These are a manifestation of the irrelevance of the Volterra cutting surface by which one can construct the defect line: a general defect line has a plastic distortion and rotation (9,10)

$$(9)\qquad \begin{cases} \partial_i u_j{}^P(\boldsymbol{x}) = \delta_i(S)(b_{\,} + \varepsilon_{jqr}\Omega_q x_r) , \\ \partial_i \omega_j{}^P(\boldsymbol{x}) = \delta_i(S)\, \Omega_j . \end{cases}$$

Changing S to S' at fixed boundary L amounts to the gauge transformation

$$(10)\qquad \begin{cases} \partial_i u_j{}^P(\boldsymbol{x}) \to \partial_i u_j{}^P(\boldsymbol{x}) + \big(\delta_i(S') - \delta_i(S)\big)(b_j + \varepsilon_{jqr}\Omega_q x_r) = \\ \qquad = \partial_i u_i{}^P(\boldsymbol{x}) + \partial_i[-\delta(V)(b_j + \varepsilon_{jqr}\Omega_q x_r)] - \varepsilon_{ijq}[-\delta(V)\,\Omega_q] , \\ \partial_i \omega_j{}^P \to \partial_i \omega_j{}^P + \partial_i[-\delta(V)\,\Omega_j] , \end{cases}$$

(7) H. KLEINERT: *Phys. Lett. A*, **95**, 381 (1983).

(8) R. D. MINDLIN: *J. Elast.*, **2**, 217 (1972); P. GERMAIN: *J. de Mec.*, **12**, 235 (1973); G. A. MAUGIN: *Acta Math.*, **35**, 1 (1980); R. A. TOUPIN: *Arch. Rat. Mech. Anal.*, **17**, 113 (1964); **11**, 385 (1962); R. D. MINDLIN and H. F. TIERSTEN: *Arch. Rat. Mech. Anal.*, **11**, 415 (1962); G. GRIOLI: *Ann. Mat. Pura Appl.*, **50**, 389 (1960); E. L. AERO and E. V. KUVSHINSKII: *Sov. Phys. Solid State*, **2**, 1272 (1961).

(9) T. MURA: *Arch. Mech.*, **24**, 449 (1972). He uses $\beta_{ij}{}^p \equiv \partial_i u_j{}^p$, $\varphi_{ij}{}^p \equiv \partial_i \omega_j{}^p$. $\varkappa_{ij}{}^p \equiv \tfrac{1}{2}\varepsilon_{ikl}\partial_l \beta_{kl}{}^p + \varphi_{ij}$.

(10) These are different from the gauge transformations of degeneracy with respect to the classical linear elasticity discussed before.

where V is the volume enclosed by the two surface shells S and S' these are obviously the continuum versions of the first two eqs. (8). Using (8), all cutting surfaces can always be gauged into certain standard configurations which then are in a one-to-one correspondence with their circumferences. An example is the axial gauge $\partial_3 u_i^P \equiv 0$, $\partial_3 \omega_i^P \equiv 0$.

For our purposes, it is the symmetric transverse gauge

$$\partial_i u_j^P(\boldsymbol{x}) \equiv \partial_j u_i^P(\boldsymbol{x}) , \qquad \partial_j \partial_j u_i^P(\boldsymbol{x}) \equiv 0 , \tag{11}$$

which will be most convenient. We can always choose the transformation functions $M_i(\boldsymbol{x})$, $N_i(\boldsymbol{x})$ such that this is satisfied (11).

This gauge simplifies drastically the coupling between the total and the plastic parts in (7). Minimizing the energy in $u_i(\boldsymbol{x})$ and using the Green's function in momentum space as

$$G_{ij}(\boldsymbol{q}) = \frac{1}{\mu \boldsymbol{q}^2(1+l^2\boldsymbol{q}^2)}\left(\delta_{ij} - \frac{q_i q_j}{\boldsymbol{q}^2}\right) + \frac{1}{(2\mu+\lambda)\boldsymbol{q}^2(1+l'^2\boldsymbol{q}^2)}\,\frac{q_i q_j}{\boldsymbol{q}^2} , \tag{12}$$

we find directly the defect energy (12)

$$\begin{aligned} E_{\text{def}} = \sum_{\boldsymbol{q}} \Bigg\{ \Big[\mu |u_{ij}^P|^2 + \frac{\lambda}{2} |u_{ll}^P|^2 \Big] &+ \tfrac{1}{2}(2\mu+\lambda) l'^2 |\partial_i u_{ll}^P|^2 + \\ &+ 2\mu l^2 \big(|\partial_i \omega_j^P|^2 + \varepsilon \partial_i \omega_j^{P*} \partial_j \omega_i^P \big) - \\ &- \tfrac{1}{2} G_{ii'}(\boldsymbol{q}) \big(\lambda \partial_i u_{ll}^P - (2\mu+\lambda) l'^2 \boldsymbol{\partial}^2 \partial_i u_{ll}^P - 2\mu l^2 \varepsilon_{ikl} \partial_l \partial_j (\partial_j \omega_k^P + \varepsilon \partial_k \omega_j^P) \big) \cdot \\ &\cdot \big(\lambda \partial_{i'} u_{ll}^P - (2\mu+\lambda) l'^2 \boldsymbol{\partial}^2 \partial_{j'} u_{ll}^P - 2\mu l^2 \varepsilon_{i'kl} \partial_l \partial_j (\partial_j \omega_k^P + \varepsilon \partial_k \omega_i^P) \big) \Bigg\} = \\ = \sum_{\boldsymbol{q}} \Bigg\{ \Big[\mu |u_{ij}^P|^2 + \frac{\lambda}{2} |u_{ll}^P|^2 \Big] &+ \frac{1}{2} \Big[(2\mu+\lambda) l'^2 q^2 - \frac{(\lambda + (2\mu+\lambda) l'^2 q^2)^2}{(2\mu+\lambda)(1+l'^2 q^2)} \Big] |u_{ll}^P|^2 + \\ &+ 2\mu l^2 \Big[(\partial_i \omega_j^P)^2 + \varepsilon \partial_i \omega_j^{P*} \partial_j \omega_i^P - \Big(1 - \frac{1}{1+l^2 q^2} \Big) \frac{q_j q_j}{q^2} \Big(\delta_{kk'} - \frac{q_k q_{k'}}{q^2} \Big) \cdot \\ &\cdot (\partial_i \omega_k^P + \varepsilon \partial_k \omega^P)(\partial_j \omega_{k'}^P + \varepsilon_i \partial_{k'} \omega_j^P) \Big] \Bigg\} . \end{aligned} \tag{13}$$

Now, all we have to do is to express the plastic distortions and rotations in terms of the defect densities η_{ij}, α_{ij}, θ_{ij}.

First of all, the defect tensor η_{ij} becomes, in the gauge (11),

$$\eta_{ij}(\boldsymbol{x}) = \partial^2(\delta_{ij} u_{ll}^P - u_{ij}^P) - \partial_i \partial_j u_{ll}^P , \tag{14}$$

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(11) In real crystals, the plastic fields are integer valued and this gauge cannot be chosen without losing this property. In the present context, however, this subtlety is irrelevant. For a proper treatment see ref. (6).

(12) Incidentally, with this method it is also easy to find a simple closed formula for the defect energy in linear elasticity crystal symmetry

$$\frac{1}{2} \sum \Big\{ c_{klk'l'} - q_j q_{j'}\, c_{ijkl} c_{i'j'k'l'} G_{ii'}(\boldsymbol{q}) \Big[\frac{1}{\boldsymbol{q}^2} (\eta_{kl} - \delta_{kl} \eta_{rr}) + \frac{q_k q_l}{\boldsymbol{q}^4} \eta_{rr} \Big] \Big[\frac{1}{\boldsymbol{q}^2} (\eta_{k'l'} - \delta_{k'l'} \eta_{r'r'}) + \frac{q_{k'} q_{l'}}{\boldsymbol{q}^4} \eta_{r'r'} \Big] \Big\} .$$

such that

$$(15)\quad \begin{cases} u_{ij}{}^P(\boldsymbol{x}) = -\dfrac{1}{\partial^2}\big(\eta_{ij} - (\delta_{ij} - \partial_j^2\,\partial_j/\partial^2)\eta_{ll}\big)\,, \\ \sum\limits_{\boldsymbol{q}} |u_{ij}{}^P|^2 = \sum\limits_{\boldsymbol{q}} \dfrac{1}{\boldsymbol{q}^4}\,|\eta_{ij}|^2\,, \qquad \sum\limits_{\boldsymbol{q}} |u_{ll}{}^P|^2 = \sum\limits_{\boldsymbol{q}} \dfrac{1}{\boldsymbol{q}^4}\,|\eta_{ll}|^2\,, \end{cases}$$

and the $u_{ij}{}^P(\boldsymbol{x})$ parts in (13) give

$$(16)\quad E_{\text{def},1} = \sum_{\boldsymbol{q}} \frac{1}{\boldsymbol{q}^4}\left[\left(\mu|\eta_{ij}|^2 + \frac{1}{2}(\lambda + (2\mu+\lambda)l'^2q^2) - \frac{(\lambda + (2\mu+\lambda)l'^2q^2)^2}{(2\mu+\lambda)(1+l'^2q^2)}\right)|\eta_{ll}|^2\right] = \\ = \sum_{\boldsymbol{q}} \frac{\mu}{\boldsymbol{q}^4}\left(|\eta_{ij}|^2 + \frac{\nu}{1-\nu}|\eta_{ll}|^2\right) + \mu l'^2 \sum_{\boldsymbol{q}} \frac{1}{\boldsymbol{q}^2(1+l'^2q^2)}\,\frac{1-2\nu}{1-\nu}\,|\eta_{ll}|^2\,,$$

where $\nu = \lambda/(2(\mu+\lambda))$ is the Poisson number.

The first term is the usual defect energy of linear elasticity which, for a special case of a pure dislocation line

$$(17)\quad \eta_{ij} = \tfrac{1}{2}\big(\varepsilon_{imn}\partial_m b_n \delta_j(L) + (ij)\big)$$

reduces to the well-known formula of Blin's [13].

Next we use (3) and find

$$(18)\quad \begin{cases} \sum\limits_{\boldsymbol{q}} |\theta_{ij}|^2 = \sum\limits_{\boldsymbol{q}} \big(|\partial_k\partial_l\omega_j{}^P|^2 - |\partial_i\partial_i\omega_j{}^P|^2\big)\,, \\ \sum\limits_{\boldsymbol{q}} |\partial_j\theta_{ij}|^2 = \sum\limits_{\boldsymbol{q}} \big(|\partial_k\partial_j\partial_l\omega_j{}^P|^2 - |\partial_l\partial_j\partial_l\omega_j{}^P|^2\big)\,, \\ \sum\limits_{\boldsymbol{q}} |\theta_{ll}|^2 = \sum\limits_{\boldsymbol{q}} \big(|\partial_k\partial_l\omega_j{}^P|^2 + 2\partial_i\partial_i\omega_j{}^{P*}\partial_k\partial_j\omega_k - \\ \qquad - \partial_k\partial_i\omega_j{}^{P*}\partial_k\partial_j\omega_i{}^P - |\partial_i\partial_i\omega_j{}^P|^2 - |\partial_j\partial_i\omega_j{}^P|^2\big)\,, \end{cases}$$

Finally, rewriting (2) as [9]

$$(19)\quad \alpha_{in} = \varepsilon_{ikl}\partial_k(u_{ln}{}^P + \varepsilon_{lnm}\omega_m{}^P) = \varepsilon_{ikl}\partial_k\partial_l u_n{}^P + \delta_{ni}\partial_k\omega_k{}^P - \partial_n\omega_i{}^P$$

and projecting out the divergenceless part of α_{in} gives

$$(20)\quad \begin{cases} \alpha^{\mathrm{T}}{}_{in} = \varepsilon_{ikl}\partial_k u_{ln}{}^P + (\delta_{in} - \hat{q}_i\hat{q}_n)\partial_l\omega_l{}^P - \partial_n\omega_i{}^P + \hat{q}_i\hat{q}_l\partial_k\omega_l{}^P\,, \\ \alpha_{ll}{}^{\mathrm{T}} = \partial_l\omega_l{}^P + \hat{q}_l\hat{q}_i\partial_l\omega_i{}^P\,, \\ \partial^2\alpha_{ll}{}^{\mathrm{T}} + \varepsilon_{kil}\partial_k\theta_{il} = -2q_lq_i\partial_l\omega_i{}^P\,, \\ \partial_i\alpha_{ij}{}^{\mathrm{T}} = -(\delta_{il} - \hat{q}_i\hat{q}_l)\partial_j\partial_j\omega_l{}^P\,. \end{cases}$$

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[13] J. Blin: *Acta Mech.*, **3**, 199 (1955).

such that the remaining pieces in (13) add up to

$$E_{\mathrm{def},2} = 2\mu l^2 \sum_{\boldsymbol{q}} \left\{ \frac{1+\varepsilon}{\boldsymbol{q}^2} |\theta_{ij}|^2 - \frac{\varepsilon}{\boldsymbol{q}^2} |\theta_{ll}|^2 - \frac{\varepsilon}{\boldsymbol{q}^4} \frac{1+\varepsilon l^2 \boldsymbol{q}^2}{1+l^2\boldsymbol{q}^2} |\partial_j \theta_{ij}|^2 + \right.$$

$$\left. + \frac{1}{1+l^2\boldsymbol{q}^2} \frac{1}{\boldsymbol{q}^2} |\partial_j \alpha_{ij}{}^{\mathrm{T}}|^2 + \frac{1+\varepsilon}{4\boldsymbol{q}^4} |\partial^2 \alpha_{ll}{}^{\mathrm{T}} + \varepsilon_{ilk} \partial_i \theta_{lk}|^2 + \frac{\varepsilon}{1+l^2\boldsymbol{q}^2} \frac{1}{\boldsymbol{q}^2} (\partial_j \alpha_{ij}{}^{\mathrm{T}*} \varepsilon_{ikl} \theta_{kl} + \mathrm{c.c.}) \right\}.$$

The energies $E_{\mathrm{def},1}$ and $E_{\mathrm{def},2}$ together are the desired total-interaction energy of the general defect line in higher-gradient elasticity. The new terms produce Biot-Savart–like forces between disclinations and local core energies for dislocations. These are sufficient to remove the above-discussed degeneracy. The new interaction energy can be used to study the statistical mechanics of ensembles of both dislocation and disclination lines ([14]). This combined study is necessary for an understanding of the melting transition via defect proliferation.

[14]) H. KLEINERT: *Phys. Lett. A*, **96**, 302 (1983).