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THE EINSTEIN-LIKE FIELD THEORY AND THE RENORMALIZATION OF THE SHEAR MODULUS

Abstract. The Einstein-like field theory is developed to describe elastic solid containing distribution of screw dislocations with finite-sized core. The core self-energy is given by the gauge-translational Lagrangian quadratic in the torsion tensor corresponding to three-dimensional Riemann–Cartan geometry. The Hilbert–Einstein gauge equation plays the role of unconventional incompatibility law. The stress tensor of the modified screw dislocations is smoothed out within the core. The renormalization of the shear modulus caused by proliferation of dipoles of non-singular screw dislocations is studied.

Dedicated to P. P. Kulish
on the occasion of his 70th birthday

§1. Introduction

The role of geometry in modern theoretical physics is considerable. The differential geometry provides framework for the analogies between the low-dimensional gravity and the defects in solids [1–4]. In turn, the multivalued fields are of great importance in the condensed matter physics to describe defects and phase transitions [5]. Multivalued gauge transformations are responsible for the topological properties of the line defects characterized by singular densities. Multivalued infinitesimal coordinate transformations for the dislocated crystals are responsible for arising of general affine spaces with curvature and torsion. It is the Riemann–Cartan geometry which is relevant to the theoretical description of solids with dislocations and disclinations [1–5].

Singularity of the dislocation densities is an idealization since the dislocation core is not captured by the classical elasticity. The translational gauge approach allows us to describe the dislocations which are non-singular due to the core regions [6, 7]. The core self-energy is given by the

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translational part of the Lagrangian advanced in [2] to describe defects in three-dimensional solids. In the case of screw dislocations, the Einstein-type gauge equation plays the role of unconventional incompatibility law. The model allows for a continuation of the classical stresses of the screw dislocation within the core, and the artificial cut-off does not occur [7]. The topological behavior of the dislocations is conventional sufficiently far from the defect lines.

Proliferation of the dislocation dipoles is responsible for the renormalization of the elastic constants [8–13] (see the review [14]). A field theory is developed in [15, 16] to describe thermodynamics of non-singular screw dislocations in elastic cylinder. The partition function of the system is considered as the functional integral. Self-energy of the dislocation cores is chosen in accordance with the gauge-translational approach [6]. Array of non-singular dislocations is equivalent to the two-dimensional Coulomb gas with smoothed out coupling. The renormalization of the shear modulus due to proliferation of dipoles of the modified screw dislocations is obtained. The influence of the dislocation cores on the renormalization of the shear modulus is demonstrated. It should be reminded that melting of two-dimensional electron crystals, [17], thermodynamics of two-dimensional Coulomb systems, [18, 19], and the dislocation-mediated melting in superfluid vortex lattices, [20], attract attention.

§2. The screw dislocations with finite-sized core

Initial and deformed states of the dislocated three-dimensional solid are described by the length elements $g_{ij}dx^i dx^j$ and $\eta_{ab}d\xi^a d\xi^b$, where the deformed state is given by the map $\mathbf{x} \longmapsto \boldsymbol{\xi}(\mathbf{x})$. The metric components are related: $\eta_{ab} = g_{ij}\mathcal{E}_a{}^i\mathcal{E}_b{}^j$, where the co-frame components $\mathcal{E}_a{}^i$ are given by 1-form $dx^i = \mathcal{E}_a{}^i dx^a$. The frame components $e^a_{\ i}$ are defined by the relation $\partial_i = e^a_{\ i}\partial_a$ (henceforth $\partial_i \equiv \partial/\partial x^i$). The components $\mathcal{E}_a{}^i$ and $e^a_{\ i}$ are orthogonal:

$$e^a_{\ i}\mathcal{E}_b{}^i = \delta^a_b, \quad e^a_{\ i}\mathcal{E}_a{}^j = \delta^j_i.$$

We consider the Eulerian strain tensor e_{ab} referred to the deformed state:

$$\eta_{ab}d\xi^a d\xi^b - g_{ij}dx^i dx^j = 2e_{ab}d\xi^a d\xi^b\,, \tag{1}$$

where

$$2e_{ab} \equiv \eta_{ab} - g_{ab}, \qquad g_{ab} \equiv g_{ij}\mathcal{B}_a{}^i\mathcal{B}_b{}^j\,. \tag{2}$$

The metric g_{ab} (2) is the Cauchy deformation tensor, and the components $\mathcal{B}_a^{\ i}$ are given by 1-form $dx^i = \mathcal{B}_a^{\ i} d\xi^a$. Assume that $\mathcal{B}_a^{\ i}$ are $\mathsf{T}(3)$-gauged:

$$\mathcal{B}_a^{\ i} = \frac{\partial x^i}{\partial \xi^a} - \varphi_a^{\ i}. \tag{3}$$

Then, dislocations are allowed provided that $\mathcal{B}_a^{\ i} d\xi^a$ is not closed due to the gauge potentials $\varphi_a^{\ i}$. The entries $\varphi_a^{\ i}$ are the translational gauge potentials, which behave under the local shifts $x^i \longrightarrow x^i + \eta^i(x)$ as follows:

$$\frac{\partial x^i}{\partial \xi^a} \longrightarrow \frac{\partial x^j}{\partial \xi^a}\Big(\delta^i_j + \frac{\partial \eta^i}{\partial x^j}\Big), \quad \varphi_a^{\ i} \longrightarrow \varphi_a^{\ i} + \frac{\partial x^j}{\partial \xi^a}\,\frac{\partial \eta^i}{\partial x^j}\,. \tag{4}$$

The transformations (4) ensure the gauge invariance of $\mathcal{B}_a^{\ i}$ (3).

The Lagrangian of the model includes, apart from non-linear elastic energy, the translational part of the eight-parameter Lagrangian $\mathcal{L}_{\rm g}$ [2], which is invariant under the coordinate shifts and local rotations. The translational part of $\mathcal{L}_{\rm g}$ depends quadratically on the torsion tensor (identified as the dislocation density) $\mathcal{T}_{ab}^{\ \ c} = (\partial_a \mathcal{B}_b^{\ i} - \partial_b \mathcal{B}_a^{\ i}) B^c_i$ (here B^c_j are reciprocals of $\mathcal{B}_a^{\ i}$):

$$\begin{aligned} \mathcal{B}^{-1}\mathcal{L}_{\rm g}\big|_{\omega=0} &= -\frac{1}{4}\mathcal{T}_{abc}(\beta_1 \mathcal{T}^{abc} + \beta_2 \mathcal{T}^{cab} + \beta_3 \mathcal{T}^{eb}_{\ \ \ e}\eta^{ac}), \\ \mathcal{B} &\equiv \det \mathcal{B}_a^{\ i}. \end{aligned}$$

Under the choice $\beta_1 = -\ell$, $\beta_2 = 2\ell$, $\beta_3 = 4\ell$, the model is governed by the Einstein-type gauge equation,

$$G^{ef} = \frac{1}{2\ell}\left(\sigma^{ef} - (\sigma_{\rm bg})^{ef}\right), \tag{5}$$

where $\boldsymbol{\sigma}$ and $\boldsymbol{\sigma}_{\rm bg}$ are the total and background stress tensors, and ℓ is the measure of the energy of the gauge field $\boldsymbol{\varphi}$. The Einstein tensor $G^{ef} \equiv \frac{1}{4}\,\mathcal{E}^{eab}\mathcal{E}^{fcd}\mathrm{R}_{abcd}$ is defined by means of the Levi–Civita tensor $\mathcal{E}^{abc}$ and the Riemann–Christoffel tensor $\mathrm{R}_{abc}^{\ \ \ \ d}$ calculated for the metric g_{ab} (2) (see [1], vol. II). The field $\boldsymbol{\sigma}_{\rm bg}$ corresponds to a prescribed distribution of the background dislocations, and $\boldsymbol{\sigma} - \boldsymbol{\sigma}_{\rm bg}$ is the driving source. The equilibrium equations are: $\overset{(\eta)}{\nabla}_a \sigma^{ab} = 0$, $\overset{(\eta)}{\nabla}_a (\sigma_{\rm bg})^{ab} = 0$, where $\overset{(\eta)}{\nabla}_a$ is the covariant derivative with respect to η_{ab}.

Non-singular screw dislocation arises in the $\mathsf{T}(3)$-gauge model proposed in [7], and its first-order stress field $\overset{(1)}{\sigma}_{\phi z}$ in the cylindrical coordinates is of the form:

$$\overset{(1)}{\sigma}_{\phi z} = -\mu \partial_\rho \overset{(1)}{\phi} = \frac{b\mu}{2\pi}\,\frac{1}{\rho}\bigl(1-\kappa\rho K_1(\kappa\rho)\bigr),$$
$$\overset{(1)}{\phi} \equiv \frac{-b}{2\pi}\bigl(\log\rho + K_0(\kappa\rho)\bigr). \tag{6}$$

Here, μ is the shear modulus, the Burgers vector component along z-axis is $b_z = b$, and $\kappa = (\mu/\ell)^{\frac{1}{2}}$. The background stress is given by $(\sigma_{\rm bg})_{\phi z} = \frac{b\mu}{2\pi}\,\frac{1}{\rho}$. The dislocation core is given by $\rho \lesssim \kappa^{-1}$, since the gauge correction to $\frac{1}{\rho}$ is exponentially small outside the core. Inside the core $\overset{(1)}{\sigma}_{\phi z} \sim \mathsf{A}\rho\log(\mathsf{B}\rho)$ at $\rho \to 0$.

§3. The renormalization of the shear modulus

The partition function $\mathcal{Z}$ of the elastic cylinder containing distribution of non-singular screw dislocations is given by the functional integral [15]:

$$\mathcal{Z} = \int e^{\beta\mathcal{L}}\,[\mathsf{Meas}]\,, \qquad \mathcal{L} \equiv \mathcal{L}_{\rm el} + \mathcal{L}_{\rm core} - i\mathcal{E}_{\rm ext}\,, \tag{7}$$

where β is inverse of the absolute temperature, and $[\mathsf{Meas}]$ is the integration measure. In framework of the plane problem of the elasticity theory, the Lagrangian $\mathcal{L}$ (7) includes the elastic contribution $\mathcal{L}_{\rm el} = \frac{-1}{2\mu}\int(\sigma_i^{\rm b}+\sigma_i^{\rm c})^2\,{\rm d}^2x$, while the other ones are:

$$\mathcal{L}_{\rm core} = \int \bigl(\ell(\partial_i e_j - \partial_j e_i)^2 + 2e_i\sigma_i^{\rm c}\bigr)\,{\rm d}^2x,$$
$$\mathcal{E}_{\rm ext} = \int \sigma_i^{\rm b}(\partial_i u - 2\mathcal{P}_i)\,{\rm d}^2x, \tag{8}$$

where $u \equiv u_3$ and $e_i \equiv e_{i3}$ are the displacement and the strain components $(i=1,2)$. The stress components $\sigma_i^{\#} \equiv \sigma_{i3}^{\#}$ are independent field variables corresponding to, so-called, *background* (# is b) or *core* (# is c) contributions. Besides, $\mathcal{P}_i$ is the plastic source which prescribes distribution of the background dislocation lines. The integration in $\mathcal{Z}$ (7) is over $\sigma_i^{\#}$, u, and e_i $(i=1,2)$.

We consider the grand-canonical ensemble of the dislocations in the *dipole phase*, which corresponds to bound pairs of the dislocations with opposite Burgers vectors ($b_z = \pm b$). Define two-point stress-stress correlation function:

$$\langle\!\langle \sigma_i(\mathbf{x}_1)\, \sigma_j(\mathbf{x}_2) \rangle\!\rangle \;=\; \mathbf{Z}^{-1}_{\rm dip} \sum_{\rm n\&p} \int \sigma_i(\mathbf{x}_1)\, \sigma_j(\mathbf{x}_2)\, e^{\beta \mathcal{L}} [\mathsf{Meas}]\,, \tag{9}$$

where $\sigma_i(\mathbf{x}) = \sigma^{\rm b}_i(\mathbf{x}) + \sigma^{\rm c}_i(\mathbf{x})$, $\mathcal{L}$ is expressed by (7), (8), and $\mathbf{Z}_{\rm dip}$ is the partition function of the array of the screw dislocations in the dipole approximation [15,16]. The functional integration in (9) is performed with a reference to a given distribution of the dislocation lines expressed by $\mathcal{P}_i$, and $\sum_{\rm n\&p}$ implies summation over number of dipoles $\mathcal{N}$, $\mathcal{N} \geqslant 1$, and averaging over their positions. The integral in right-hand side of (9) is calculated in [15], and the correlator in the dipole representation of the Coulomb gas is obtained:

$$\begin{aligned} \langle\!\langle \sigma_i(\mathbf{x}_1) \sigma_j(\mathbf{x}_2) \rangle\!\rangle &= \frac{-\mu}{2\pi\beta}\, \partial_{(\mathbf{x}_1)_i} \partial_{(\mathbf{x}_2)_j} \mathcal{U}(\kappa|\mathbf{x}_1 - \mathbf{x}_2|) \\ &\quad + \mathbf{Z}^{-1}_{\rm dip} \sum_{\rm n\&p} \sigma_i(\mathbf{x}_1) \sigma_j(\mathbf{x}_2)\, e^{-\beta \mathcal{W}_{\rm dip}}, \\ \mathcal{U}(s) &\equiv \log\bigl(\frac{\gamma}{2} s\bigr) + K_0(s), \end{aligned} \tag{10}$$

where $\sigma_i = \mu \epsilon_{ik}\, \partial_{x_k} \phi$, and $\phi \equiv \overset{(1)}{\phi}$ is the stress potential of superposition of $\mathcal{N}$ dipoles. Positions of dipoles are confined within a disk of radius R.

The energy $\mathcal{W}_{\rm dip}$ in (10) arises, [16], in the dipole approximation from the effective energy $\mathcal{W}$ of $2\mathcal{N}$ non-singular screw dislocations with unit Burgers vectors ($b = 1$):

$$\mathcal{W} = \frac{-\mu}{4\pi} \sum_{I,J} \bigl(\mathcal{U}(\kappa|\mathbf{y}^+_I - \mathbf{y}^+_J|) + \mathcal{U}(\kappa|\mathbf{y}^-_I - \mathbf{y}^-_J|) - 2\mathcal{U}(\kappa|\mathbf{y}^+_I - \mathbf{y}^-_J|) \bigr), \tag{11}$$

where $\mathcal{U}(s)$ is given by (10). Due to condition of "electro-neutrality", the number of positive dislocations at the points $\{\mathbf{y}^+_I\}_{1 \leqslant I \leqslant \mathcal{N}}$ is equal to the number of negative ones at the points $\{\mathbf{y}^-_I\}_{1 \leqslant I \leqslant \mathcal{N}}$. The energy $\mathcal{W}$ (11) demonstrates that the array of the modified screw dislocations is equivalent to the two-dimensional Coulomb gas of unit charges ± 1 characterized by the two-body potential $\mathcal{U}$ (10) which is logarithmic at large separation but tends to zero for the charges sufficiently close to each other.

The stress-stress correlator $\langle\!\langle \sigma_i(\mathbf{x}_1)\, \sigma_j(\mathbf{x}_2) \rangle\!\rangle$ given by (10) is calculated in [16] with respect of the dipole-dipole coupling. It is given with leading logarithmic accuracy:

$$\langle\!\langle \sigma_i(\mathbf{x}_1)\,\sigma_j(\mathbf{x}_2)\rangle\!\rangle \approx \frac{-\mu}{2\pi\beta}\Big(\partial_{(\mathbf{x}_1)_i}\partial_{(\mathbf{x}_2)_j}\mathcal{U}(\kappa|\Delta\mathbf{x}|)+ \\ +\epsilon_{ik}\epsilon_{jl}\,\partial_{(\mathbf{x}_1)_k}\partial_{(\mathbf{x}_2)_l}\frac{\beta\mu d\,\mathcal{U}(\kappa|\Delta\mathbf{x}|)+\log(1+\beta\mu d)\,\mathsf{D}_\kappa K_0(\kappa|\Delta\mathbf{x}|)}{1+\beta\mu d}\Big)\,, \tag{12}$$

where $\Delta\mathbf{x} \equiv \mathbf{x}_1 - \mathbf{x}_2$, $\partial_{\mathbf{x}} \equiv (\partial_{x_1}, \partial_{x_2})$, D_κ stands for $\frac{-\kappa}{2}\frac{\mathrm{d}}{\mathrm{d}\kappa}$, and d is proportional to mean area covered by the dipoles.

We consider the renormalization of the shear modulus μ caused by proliferation of the dislocation dipoles. The renormalized μ_{ren} is defined as follows [8, 10, 11, 13]:

$$\frac{1}{\mu_{\mathrm{ren}}} \equiv \frac{\beta}{\mu^2\mathcal{S}}\sum_{i,k=1,2}\iint\langle\!\langle\sigma_i(\mathbf{x}_1)\,\sigma_k(\mathbf{x}_2)\rangle\!\rangle\,\mathrm{d}^2\mathbf{x}_1\mathrm{d}^2\mathbf{x}_2\,, \tag{13}$$

where $\mathcal{S}$ is the cross-section area. Using $\langle\!\langle\sigma_i(\mathbf{x}_1)\,\sigma_k(\mathbf{x}_2)\rangle\!\rangle$ (12) in (13), one obtains:

$$\frac{\mu}{\mu_{\mathrm{ren}}} = \frac{(1+2\beta\mu d)\,\mathcal{C}_1(\kappa R) - \log(1+\beta\mu d)\,\mathcal{C}_{\mathsf{D}}(\kappa R)}{1+\beta\mu d}\,, \tag{14}$$

where $\mathcal{C}_1$ and $\mathcal{C}_{\mathsf{D}}$ are given by the modified Bessel functions,

$$\begin{aligned}\mathcal{C}_1(z) &= 1 - 2K_1(z)I_1(z)\,,\\ \mathcal{C}_{\mathsf{D}}(z) &= -\mathsf{D}_z\mathcal{C}_1(z) \;=\; -1 + zI_1(z)(K_0(z)+K_2(z))\,.\end{aligned} \tag{15}$$

Equation (14) enables us to express the renormalized shear modulus as the function of temperature, $\mu_{\mathrm{ren}} = \mu_{\mathrm{ren}}(T)$, below the melting temperature $T_c = \frac{\mu}{8\pi}$, [15, 16].

The renormalized shear modulus μ_{ren} (14) depends on the ratio $R/\kappa^{-1} = \kappa R$ of two lengths characterizing the cylinder cross-section and the dislocation core. The dependence on κR displays the effect of the unconventional dislocation solution on the shear modulus near the melting transition. Recall that properly rescaled Young modulus tends to 16π at $T \to T_c^-$ according to the theory developed in [9–13]. This universality is crucial for singular defects, and it is also discussed in [1]. A confirmation of this fact for two-dimensional colloidal crystals has been reported in [21]. The approach [16] demonstrates that the limiting value of the renormalized shear modulus deviates from a multiple of π due to the peculiar singularityless character of the dislocations:

$$\frac{\mu_{\rm ren}(T_c^-)}{T_c} \approx \frac{8\pi}{\mathcal{C}_1(\kappa R)} \xrightarrow[\kappa R \gg 1]{} 8\pi\,, \qquad d \ll 1\,. \tag{16}$$

The results obtained should be applicable to nanotubes and nanowires with comparable R and κ^{-1}. Further development for nonsingular edge dislocations seems to be interesting as far as multi-layer nanotubes and wrapped crystals are concerned. It should also be noticed that the melting criteria of two-dimensional systems are still actively discussed [22, 23].

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