# ПРЕПРИНТЫ ПОМИ РАН



Учредитель: Санкт-Петербургское отделение Математического института им. В. А. Стеклова Российской академии наук

Свидетельство о регистрации средства массовой информации: ЭЛ №ФС 77-33560 от 16 октября 2008 г. Выдано Федеральной службой по надзору в сфере связи и массовых коммуникаций

Контактные данные: 191023, г. Санкт-Петербург, наб. реки Фонтанки, дом 27

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http://www. pdmi.ras.ru /preprint/

Заведующая информационно-издательским сектором Симонова В.Н

PDMI preprint 10/2010

# On equivalence of ensemble of non-singular screw dislocations to a Coulomb-like gas with smoothed out coupling

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**Abstract**

A field theory is developed for a thermodynamical description of array of parallel non-singular screw dislocations in continuous elastic body. The partition function of the system is considered in the functional integral form. Expression for the self-energy of the dislocation cores is proposed in the form suggested by the gauge-translational model of non-singular screw dislocation. It is shown that the system of the dislocations at large mutual separations is equivalent to the two-dimensional Coulomb gas of charges interacting logarithmically. The coupling potential is prevented from a short-distance divergency since the core energies are taken into account. Analogue of the "electro-neutrality" condition reduces the system to a collection of the dislocation dipoles. Two-point correlation functions of the stress components are obtained. The law of renormalization of the shear modulus due to the presence of the dislocations is considered in the approximation of non-interacting dipoles. It is demonstrated that the finite size of the dislocation cores causes modification of the renormalization law.

**Key words:** functional integration, dislocation, Coulomb gas, renormalization

# ПРЕПРИНТЫ

**Санкт-Петербургского отделения**

**Математического института им. В. А. Стеклова**

**Российской академии наук**

**PREPRINTS**

**of the St.Petersburg Department of Steklov Institute of Mathematics**

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# 1 Introduction

Topologically non-trivial configurations, such as vortices, dislocations, and other defects, occurring in ordered states attract appreciable attention in modern condensed matter physics. For instance, dislocations as imperfections of the crystalline ordering are of importance for structural, transport, and electronic properties of real solids. It is widely recognized after the pioneer works [1–6] that the two-dimensional ordered states are of special interest due to significance of the defects for the corresponding phase transitions. The ideas [1–6] have been further elaborated for description of the dislocation-mediated crystal melting in two dimensions [7–11]. In their turn, the textbooks [12–14] summarize an original field-theoretical approach to the ordered states and phase transitions dominated by the line-like disturbances. The peculiarity of [12–14] is due to a systematical usage of (singular) gauge fields. Certain aspects of the statistical physics of the dislocation arrays, as well as appropriate correlation functions, are considered in [15–18].

Dislocations have recently attracted considerable attention concerning the physics of carbon and noncarbon nanotubes [19–22]. In particular, multilayer nanotubes can contain within their walls screw dislocations lying along the tube axis [21]. Therefore influence of the dislocation cores can become important provided the core sizes are not negligible in comparison with thickness of the tube walls. Notice that the electronic properties of the graphene sheets in presence of dislocations are also of interest in the context of nanotubes [23].

The topological nature of a single dislocation is manifested through its stress tensor components displaying singularity on the defect line. In reality, the stress components are smoothed out within the core regions. Since the first attempts [24, 25], various approaches to the dislocations with non-trivial core are known. For instance, the quasi-continuum approach [26, 27], the gradient elasticity [28, 29], and the Lagrangian translational gauging [31–34] enable to obtain continuous models of non-singular screw dislocation.

Crucially, the elastic stresses of the screw dislocation are obtained in [31–34] in the form of superposition of conventional far-reaching ("background") contribution and short-ranged ("gauge") correction which modifies the "background" stresses within a compact core. Therefore the gauge Lagrangians [31–34] allow to cancel the singularity of the conventional screw dislocation thus leading to so-called *modified* screw dislocation. Notice that the second-order elasticity is of importance for the defects in crystals [35]. The approach [32] admits of extension to the case of second order corrections [36].

The present paper is concerned with a thermodynamical ensemble of the modified screw dislocations [32] lying within a long enough rod of circular cross-section. The functional integration [14, 37–40] is used to represent the partition function and to study certain thermodynamical averages for the system in question. The core energies are accounted for in the way [32] so that the modified screw dislocation plays a role of the stationarity point of appropriate functional integral (obtaining of the dislocation core energies from the first principle calculations also attracts attention [41]). It is shown that the collection of parallel non-singular dislocations is equivalent to the two-dimensional Coulomb-like system of charges interacting *via* the potential which is logarithmic at large distances but vanishes locally (smoothed out coupling). Remind that the two-dimensional Coulomb gas [42] belongs to the class of systems covered by [1–6] and has a relationship with the two-dimensional spin models [43, 44].

Dislocations available in a solid sample result in renormalization of the values of the corresponding elastic moduli [9, 16]. Appropriate two-point correlation functions of the stress components are calculated below by means of the method of generating functional (introduced to statistical mechanics in [45,46]) in order to investigate the renormalization of the shear modulus. It is demonstrated that non-triviality of the core results in a correction to the law of renormalization of the shear modulus what could be appreciable for nanotubes. The present field-theoretical approach is influenced technically by that of Ref. [47], where certain correlation functions have been calculated for the string models possessing the world-sheet vortices.

The paper is organized as follows. Section 1 is introductive. Section 2 deals with the partition function, and transformation of collection of the dislocation dipoles to a dual system of pairs of two-dimensional charges is presented. Section 3 provides estimations for certain thermodynamical averages, e.g., for the average square of the dislocation dipole momentum and for the stress-stress correlation function in the approximation of non-interacting dipoles. The renormalization of the shear modulus in presence of non-singular dislocations is considered. Discussion in Section 5 concludes the paper.

# 2 The partition function

Consider a cylindric rod containing array of non-singular screw dislocations which are parallel to the cylinder axis. The cylinder's material is approximated by elastically-isotropic continuum described by linear elasticity. Remind that the screw dislocation is characterized by parallelism between its Burgers vector and tangent to the dislocation line [48]. The modified screw dislocation [32] is a point of departure of the present investigation which treats the array of the dislocations as a thermodynamical ensemble at non-zero temperature. The functional integration approach is used below to represent the partition function and certain correlation functions of the collection of non-singular screw dislocations. In what follows, the Cartesian axis $Ox_3$ is along the cylinder's axis.

Let us begin with the thermodynamical partition function $\mathcal{Z}$ of the elastic cylinder containing the dislocations which is expressed in the form of the functional integral:

$$\mathcal{Z} = \frac{1}{N} \int e^{-\beta W}\, \mathcal{D}(\sigma^{\rm b}_{ij}, \sigma^{\rm c}_{ij}, u_i, e_{ij})\,, \tag{1}$$

$$W \equiv E - \frac{i}{\beta} E_{\rm ext}\,, \qquad E \equiv E_{\rm el} + E_{\rm core}\,, \tag{2}$$

where $\beta$ is inverse of the absolute temperature $T$ (the Boltzmann constant is unity). The functional $W$ (2) is expressed by the following contributions (indices repeated imply summation):

$$\begin{aligned}
E_{\rm el} &= \frac{1}{4\mu} \int \Bigl( (\sigma^{\rm b}_{ij} + \sigma^{\rm c}_{ij})^2 - \frac{\nu}{1+\nu} (\sigma^{\rm b}_{ii} + \sigma^{\rm c}_{ii})^2 \Bigr)\, {\rm d}^3 x\,, \\
E_{\rm core} &= \int \bigl( \ell\, e_{ij} ({\rm inc}\, e)_{ij} \,-\, e_{ij}\, \sigma^{\rm c}_{ij} \bigr)\, {\rm d}^3 x\,, \\
E_{\rm ext} &= \frac{1}{2} \int \sigma^{\rm b}_{ij} (\partial_i u_j + \partial_j u_i - 2\mathcal{P}_{ij})\, {\rm d}^3 x\,.
\end{aligned} \tag{3}$$

The functional $E_{\rm el}$ (3) is the elastic energy of superposition of two stresses, $\sigma^{\rm b}_{ij}$ and $\sigma^{\rm c}_{ij}$, provided $\mu$ and $\nu$ are respectively identified as the shear modulus and the Poisson ratio. The notation $\sigma^{\rm b}_{ij}$ is reserved for the long-ranged contribution, while the term $\sigma^{\rm c}_{ij}$

describes a non-conventional stress which modifies the background one, $\sigma^{\mathrm{b}}_{ij}$, within the core of the modified dislocation [32] [1]. The functional $E_{\mathrm{core}}$ (3) is the dislocation core energy. The contribution $e_{ij}(\mathrm{inc}\, e)_{ij}$ in it originates (by means of linearizations) from the Hilbert–Einstein gauge Lagrangian proposed in [32] in framework of the translational gauge approach to dislocations [2]. Here the double-curl operator acts on the total strain tensor $e_{ij}$: $(\mathrm{inc}\, e)_{ij} \equiv -\epsilon_{ikl}\epsilon_{jmn}\partial_k\, \partial_m e_{ln}$ ($\epsilon_{ikl}$ is totally antisymmetric tensor) [54]. The parameter $\ell$ characterizes a scale of the dislocation core energy. The term $E_{\mathrm{ext}}$ (3) is linear with respect of (symmetrized) derivatives of the displacement vector $u_i$, as well as with respect of a "source" $\mathcal{P}_{ij}$ which is related to the plastic strain $e^P_{ij}$ as follows: $\mathcal{P}_{ij} = e^P_{ij} + C_{ij}$. Specific configuration of singular dislocation lines is prescribed by appropriately chosen $e^P_{ij}$ since the plastic strain is concentrated on cut surfaces bounded by the dislocation lines [55]. The present approach enables to avoid the stress divergencies on the dislocation lines. Therefore an auxiliary field $C_{ij}$ (which is not a functional variable) is postulated which allows to fix the background so that the tensor field $\sigma^{\mathrm{b}}_{ij}$ just coincides with the classical dislocation stresses governed by $e^P_{ij}$ ($C_{ij} = 0$ at $\ell = 0$).

The notation $\mathcal{D}(\sigma^{\mathrm{b}}_{ij}, \sigma^{\mathrm{c}}_{ij}, u_i, e_{ij})$ implies in (1) the integration measure equal to a product of measures corresponding to each functional variable inside the brackets. More details on definition of the functional integration measure by means of appropriate limiting procedure can be found in [37–39]. The normalization factor $1/N$ is to absorb physically irrelevant multiplicative infinities. It is the present choice of Eqs.(2), (3) which enables a collection of the modified screw dislocations [32] to provide an extremum of the functional $W$.

Our framework is that of the plane elasticity. Thus it is assumed that the cylinder containing the dislocations is long enough and influence of its ends is negligible [48, 57]. The independence on the third coordinate reduces our study to two dimensions. Therefore the functionals (3) take the form:

$$
\begin{aligned}
L^{-1}E_{\mathrm{el}} &= \frac{1}{2\mu}\int (\sigma^{\mathrm{b}}_i + \sigma^{\mathrm{c}}_i)^2\, \mathrm{d}^2x\,, \\
L^{-1}E_{\mathrm{core}} &= 2\int (\ell\, e_i(\mathrm{inc}\, e)_i \,-\, e_i\, \sigma^{\mathrm{c}}_i)\, \mathrm{d}^2x\,, \\
L^{-1}E_{\mathrm{ext}} &= \int \sigma^{\mathrm{b}}_i(\partial_i u - 2\mathcal{P}_i)\, \mathrm{d}^2x\,,
\end{aligned}
\tag{4}
$$

where the integrands are $(x_1, x_2)$-dependent, and the summation goes over $i = 1, 2$. Since the displacement vector of straight screw dislocation is along $Ox_3$ [48], we use $u \equiv u_3$. Besides, we use the abbreviations: $\sigma^{\#}_i \equiv \sigma^{\#}_{i3}$ ($\#$ is b or c), $e_i \equiv e_{i3}$, etc. (the same convention is for 'inc'). Appropriate specification of the functional integration measure should be expressed as $\mathcal{D}(\sigma^{\mathrm{b}}_i, \sigma^{\mathrm{c}}_i, u, e_i)$. Besides, a length $L$ is introduced to keep the dimensionality.

First, the following notice concerning $\mathcal{Z}$ (1) should be made provided three-dimensional Eqs. (3) are used at $\ell = 0$. Shifting subsequently the integration variables $\sigma^{\mathrm{c}}_{ij} \to \sigma^{\mathrm{c}}_{ij} + \hat{\sigma}_{ij}$

[1]Two stress fields $\sigma^{\mathrm{b}}_{ij}$ and $\sigma^{\mathrm{c}}_{ij}$ correspond to subdivision of the total elastic stress into, so-called, "background" and "gauge" parts [31–34].

[2]The gauge Lagrangians quadratic in the dislocation densities are used in [31,33] what is equivalent, in the case of the screw dislocation, to the approach of [32]. The most general gauge Lagrangian for three-dimensional space has been discussed in [49]. Certain developments in the gauge gravity demonstrate (see [13, 50–53]) the gauge-translational features of the theory of dislocations.

and $e_{ij} \rightarrow e_{ij} + \hat{e}_{ij}$ (where $\hat{\sigma}_{ij}$ and $\hat{e}_{ij}$ are new adjustable fields), it is possible to remove in $E$ the terms linear in $\sigma^{\rm c}_{ij}$ and $e_{ij}$. Then, the integrations over $\sigma^{\rm c}_{ij}$ and $e_{ij}$ are decoupled and can be compensated by redefinition of $1/N$. Eventually, $E$ is reduced to $E_{\rm el} = E_{\rm el}(\sigma^{\rm b}_{ij})$, and two remaining integrations, over $u$ and $\sigma^{\rm b}_{ij}$, result (in agreement with [12–14]) in the partition function of array of singular dislocations characterized by a specific choice of $e^P_{ij}$.

Let us go over to Eqs. (4) at $\ell = 0$. The source $\mathcal{P}_i$ is taken at $\ell = 0$ in the form: $\mathcal{P}_i = e^P_i$. A single positively oriented straight screw dislocation intersecting the plane $x_1Ox_2$ at $\mathbf{x} = \mathbf{y}$ (we use $\mathbf{x} \equiv (x_1, x_2)$) is "produced" by the plastic strain with a single non-zero component $e^P_2 = (b/2)\theta(-x_1 + y_1)\delta(y_2 - x_2)$ [55]. Here $\theta(\cdot)$ is the Heaviside function and $b$ is absolute value of the Burgers vector $\mathbf{b}$ lying along $Ox_3$. Further, the integration over $u$ is equivalent to insertion of the delta-like functional $\delta(\partial_i\sigma^{\rm b}_i)$. The equilibrium equation $\partial_i\sigma^{\rm b}_i = 0$ is fulfilled by the Kröner ansatz $\sigma^{\rm b}_i \equiv \mu\, \epsilon_{ij}\, \partial_j f^{\rm b}$, where $\epsilon_{ij}$ is totally antisymmetric symbol of second rank [54]. Vanishing of the variation $\delta W$ under the variation $f^{\rm b} \rightarrow f^{\rm b} + \delta f^{\rm b}$ allows to determine the potential $f^{\rm b}$.

Consider a pair of two screw dislocations with the coordinates $\mathbf{x} = \mathbf{y}_1$ and $\mathbf{x} = \mathbf{y}_2$ and with the Burgers vectors $\mathbf{b}_1$ and $\mathbf{b}_2$, respectively. Assume that the boundary of the bulk consists of the cylinder's outer surface and of a set of cylindric tubes which enclose each dislocation line. Indeed, a cut-off at small distance from the dislocation line is inevitable, since the dislocation core is not captured at $\ell = 0$. It is appropriate to require that the variation $\delta f^{\rm b}$, as well as its derivative $\frac{\partial}{\partial n}(\delta f^{\rm b})$ in direction normal to the boundary, both are vanishing on each component of the boundary of the cylinder's cross-section. Taking into account the vanishing requirements, we obtain the extremum condition:

$$\Delta f^{\rm b} \;=\; \frac{2i}{\beta}\,(\partial_1 e^P_2 \;-\; \partial_2 e^P_1) \;=\; \frac{-i}{\beta}\big(b_1 \overset{(2)}{\delta}(\mathbf{x} - \mathbf{y}_1) + b_2 \overset{(2)}{\delta}(\mathbf{x} - \mathbf{y}_2)\big)\,, \tag{5}$$

where $\overset{(2)}{\delta}(\mathbf{x})$ is two-dimensional delta-function on $x_1Ox_2$, and $b_1$, $b_2$ are absolute values of the Burgers vectors. We determine $f^{\rm b}$ from (5) as follows:

$$f^{\rm b} \;=\; \frac{i}{\beta} f_P\,, \qquad f_P \equiv \frac{-1}{2\pi}\,(b_1 \log|\mathbf{x} - \mathbf{y}_1| + b_2 \log|\mathbf{x} - \mathbf{y}_2|)\,, \tag{6}$$

where $f_P$ is the Prandtl stress potential [54] of two screw dislocations.

Now let us turn to $\ell \neq 0$ and require vanishing of $\delta W$ under independent variations of its functional arguments. The variation of $\sigma^{\rm c}_{ij}$ results in the 'strain–stress' constitutive law

$$e_{ij} \;=\; \frac{1}{2\mu}\Big(\sigma^{\rm b}_{ij} + \sigma^{\rm c}_{ij} - \frac{\nu}{1+\nu}\big(\sigma^{\rm b}_{ll} + \sigma^{\rm c}_{ll}\big)\delta_{ij}\Big)\,, \tag{7}$$

and the variation of $e_{ij}$ gives the equation:

$$({\rm inc}\, e)_{ij} \;=\; \frac{1}{2\ell}\,\sigma^{\rm c}_{ij}\,. \tag{8}$$

Since $\partial_i({\rm inc}\, e)_{ij} \equiv 0$, we put $\sigma^{\rm c}_i = \mu\, \epsilon_{ij}\, \partial_j f^{\rm c}$ in order to fulfil $\partial_i\sigma^{\rm c}_i = 0$. It is assumed that the variations $\delta f^{\rm b}$ and $\delta f^{\rm c}$ are vanishing on the external cylinder's boundary. The same is true for their normal derivatives. Using Eqs. (5)–(8), one obtains the extremum conditions:

$$\begin{aligned} \Delta\big(f^{\rm b} + f^{\rm c}\big) \;&=\; \frac{2i}{\beta}\,(\partial_1\mathcal{P}_2 \;-\; \partial_2\mathcal{P}_1)\,, \\ \Delta\big(f^{\rm b} + f^{\rm c}\big) \;&=\; \kappa^2 f^{\rm c}\,, \qquad \kappa^2 \equiv \frac{\mu}{\ell}\,, \end{aligned} \tag{9}$$

where $\mathcal{P}_i \equiv e_i^P + C_i$. Self-consistency of equations (9) requires coincidence of their right-hand sides and takes the form:

$$\partial_1 C_2 \,-\, \partial_2 C_1 \,=\, \frac{\beta}{2i}\,\kappa^2 f^{\rm c} \,+\, \frac{1}{2}\big(b_1 \overset{(2)}{\delta}(\mathbf{x}-\mathbf{y}_1) + b_2 \overset{(2)}{\delta}(\mathbf{x}-\mathbf{y}_2)\big)\,. \tag{10}$$

Analytical form of $C_i$ results from general solution to (10):

$$C_i \,=\, \frac{\beta}{2i}(\partial_i\phi \,-\, \epsilon_{ij}\,\partial_j\psi)\,, \tag{11}$$

where $\phi$ is arbitrary regular function, while $\psi$ is to be found after substitution of (11) to (10). Provided (10) is respected, either $f^{\rm b}$ or $f^{\rm c}$ can be fixed arbitrarily. Our strategy is to keep $f^{\rm b}$ still respecting Eq. (5) at $\ell \neq 0$. Then Eqs. (9) lead to a single equation for $f^{\rm c}$:

$$(\Delta \,-\, \kappa^2) f^{\rm c} \,=\, \frac{i}{\beta}\big(b_1 \overset{(2)}{\delta}(\mathbf{x}-\mathbf{y}_1) + b_2 \overset{(2)}{\delta}(\mathbf{x}-\mathbf{y}_2)\big)\,, \tag{12}$$

which is solved as follows:

$$f^{\rm c} \,=\, (i/\beta) f_K\,, \qquad f_K \,=\, \frac{-1}{2\pi}\,(b_1 K_0(\kappa|\mathbf{x}-\mathbf{y}_1|) \,+\, b_2 K_0(\kappa|\mathbf{x}-\mathbf{y}_2|))\,, \tag{13}$$

where $K_0(\cdot)$ is the modified Bessel function. Besides, the choice $\phi = 0$, $\psi = f^{\rm c}$ ensures that Eqs. (10) and (12) are coinciding.

Therefore, the whole potential $f^{\rm b} + f^{\rm c} = (i/\beta)(f_P + f_K)$ describes a couple of non-singular screw dislocations. Notice that the fields $\sigma_i^{\rm b}$ and $\sigma_i^{\rm c}$ are rather the stationarity solutions of the functional $W$ (2), while the proper stress fields are given by $\frac{\beta}{i}\,\sigma_i^{\rm b}$ and $\frac{\beta}{i}\,\sigma_i^{\rm c}$. Equations (6) and (13) demonstrate that a modification of the conventional (Prandtl) stress potential $f_P$ occurs within the core regions, i.e., within the tubular vicinities of transverse size $\simeq \kappa^{-1}$ (the length $\kappa^{-1}$ should not, in principle, be the same as the lattice spacing). When $\kappa|\mathbf{x}-\mathbf{y}_{1,2}| \gg 1$, the total solution is dominated by the conventional contribution $f^{\rm b}$. When either $\kappa|\mathbf{x}-\mathbf{y}_1| \ll 1$ or $\kappa|\mathbf{x}-\mathbf{y}_2| \ll 1$, the sum $f^{\rm b} + f^{\rm c}$ behaves smoothly at $\mathbf{x} \to \mathbf{y}_{1,2}$, and the known singularities in the total stress distribution $\frac{\beta}{i}\,(\sigma_i^{\rm b} + \sigma_i^{\rm c})$ do not appear.

To sum up, the variational approach gave a couple of the modified screw dislocations [32]. Remind that the modified screw dislocation [32] agrees with the solution obtained by means of the gradient elasticity [29,30]. The gradient elasticity itself belongs to a class of the generalized continuum theories which effectively take into account interatomic forces in order to explain the material behavior on the nano-scales (and thus inside the defect cores) [56]. The solution obtained will be used for the stationary phase estimation of the functional integral in question.

Let us estimate the partition function given by (1), (2) and (4) using the stationary phase method [37–39]. Integration by parts transforms $e_i(\mathrm{inc}\,e)_i$ in $W$ into the quadratic expression: $-\frac{1}{2}(\partial_i e_j \,-\, \partial_j e_i)^2$. It is invariant under the shift $e_i \,\to\, e_i \,+\, \partial_i g$, where $g$ is an arbitrary function (the Abelian gauge transformation). It is necessary to restrict the functional integration over $e_i$ by imposing, say, the "Coulomb gauge" $\partial_i e_i = 0$. This procedure is widely known as the 'Faddeev–Popov trick' [37]. Eventually, the contribution $\ell e_i(\mathrm{inc}\,e)_i$ in $W$ is replaced by $\ell e_i \Delta e_i$. The shift of the integration variable,

$$e_i \,\to\, e_i \,+\, (2\ell)^{-1}\,\Delta^{-1}\sigma_i^{\rm c}\,, \tag{14}$$

cancels the term linear in $e_i$ (the gauge condition is respected due to $\partial_i \sigma_i^{\mathrm{c}} = 0$). Here $\Delta^{-1}$ is the operator of convolution, and its kernel is given by the Green function of two-dimensional Laplacian. The resulting Gaussian integration over $e_i$,

$$\int e^{-2\ell\beta L \int e_i \Delta e_i \, \mathrm{d}^2 x} \mathcal{D}(e_i)\,,$$

is absorbed into $1/N$, and the partition function $\mathcal{Z}$ takes the form:

$$\mathcal{Z} \;=\; \frac{1}{N} \int e^{-\beta \widetilde{\widetilde{W}}} \mathcal{D}(\sigma_i^{\mathrm{b}}, \sigma_i^{\mathrm{c}}, u)\,, \tag{15}$$

$$\widetilde{\widetilde{W}} \;\equiv\; \widetilde{E} \;-\; \frac{i}{\beta} E_{\mathrm{ext}}\,, \quad \widetilde{E} \equiv E_{\mathrm{el}} + \widetilde{E}_{\mathrm{core}}\,, \tag{16}$$

where the source $E_{\mathrm{ext}}$ is given by (4), and $\widetilde{E}_{\mathrm{core}}$ is expressed as follows:

$$L^{-1} \widetilde{E}_{\mathrm{core}} \;\equiv\; \frac{-1}{2\ell} \int \sigma_i^{\mathrm{c}} \, \Delta^{-1} \sigma_i^{\mathrm{c}} \, \mathrm{d}^2 x\,. \tag{17}$$

The functional $\widetilde{\widetilde{W}}$ includes the elastic energy of two non-singular dislocations, $E_{\mathrm{el}}$, while the (localized) core energies are given by (17). The representations expressed either by (1), (2) or by (15), (16) are equivalent, i.e., the same Eqs. (5) and (9) arise for $f^{\mathrm{b}}$ and $f^{\mathrm{c}}$, respectively, provided vanishing of $\delta f^{\mathrm{b}}$ and $\delta f^{\mathrm{c}}$ is properly required.

Let us estimate (15) by the stationary phase approximation. First, we obtain:

$$\begin{aligned} L^{-1} \widetilde{E} \;=\; \frac{-\mu}{2}\, \kappa^2 \Big[ \int f^{\mathrm{c}} f^{\mathrm{b}} \, \mathrm{d}^2 x \;-\; \kappa^{-2} \oint \big(f^{\mathrm{b}} + f^{\mathrm{c}}\big) \frac{\partial}{\partial n} \big(f^{\mathrm{b}} + f^{\mathrm{c}}\big) \, \mathrm{d}s \\ + \oint f^{\mathrm{c}} \frac{\partial}{\partial n} \big(\Delta^{-1} f^{\mathrm{c}}\big) \, \mathrm{d}s \Big]\,, \end{aligned} \tag{18}$$

where the Green theorem is used. The contour integrations in (18) are along the outer boundary and the circles of small radius $\epsilon$ around the dislocations. It is appropriate to renormalize the integration variables in (15) so that $f^{\mathrm{b}} \to (1/\beta) f^{\mathrm{b}}$, $f^{\mathrm{c}} \to (1/\beta) f^{\mathrm{c}}$. Using again Eqs. (5), (9), we formally express (in the renormalized terms):

$$\int f^{\mathrm{c}} f^{\mathrm{b}} \, \mathrm{d}^2 x \;=\; 4 \int \partial_1 e_2^P(\mathbf{x})\, \Delta^{-1} (\Delta - \kappa^2)^{-1} \, \partial_1 e_2^P(\mathbf{s}) \, \mathrm{d}^2 x \, \mathrm{d}^2 s\,, \tag{19}$$

where the convolution of two Green functions of the corresponding operators $\Delta$ and $\Delta - \kappa^2$ depends on the difference $\mathbf{x} - \mathbf{s}$. Recall that expression for the plastic source of the couple of dislocations reads:

$$\partial_1 e_2^P(\mathbf{s}) = \frac{-1}{2} \sum_{k=1}^{2} b_k \overset{(2)}{\delta} (\mathbf{s} - \mathbf{y}_k)\,.$$

We estimate right-hand side of (19) and obtain after the limit $\epsilon \to 0$:

$$\begin{aligned} \kappa^2 \int f^{\mathrm{b}} f^{\mathrm{c}} \, \mathrm{d}^2 x \;=\; \frac{b_1^2 + b_2^2}{2\pi} \log\big(\frac{\gamma}{2}\kappa\big) - \\ - \frac{b_1 b_2}{\pi} \big(K_0(\kappa |\mathbf{y}_1 - \mathbf{y}_2|) \;+\; \log |\mathbf{y}_1 - \mathbf{y}_2|\big) \;+\; \mathcal{O}(e^{-\kappa R})\,, \end{aligned} \tag{20}$$

$$\oint \big(f^{\mathrm{b}} + f^{\mathrm{c}}\big) \frac{\partial}{\partial n} \big(f^{\mathrm{b}} + f^{\mathrm{c}}\big) \, \mathrm{d}s \;=\; -\, \frac{(b_1 + b_2)^2}{2\pi} \log R \;+\; \mathcal{O}\big(\frac{|\mathbf{y}_{12}|}{R},\, e^{-\kappa R}\big)\,, \tag{21}$$

where $\mathcal{O}(e^{-\kappa R})$ implies negligible contributions due to the external boundary. The notation $\mathcal{O}\big(\frac{|\mathbf{y}_{12}|}{R},\,\cdot\big)$ in (21) stands for the contributions, which are unimportant provided $|\mathbf{y}_{12}| \equiv |\mathbf{y}_1 - \mathbf{y}_2|$ is not too large with respect to $R$. The third integral in (18) is estimated as $\mathcal{O}(e^{-\kappa R})$. Further, estimation of the term $\frac{-i}{\beta}E_{\rm ext}$ demonstrates that the absolute value of its leading part is greater twice than that of $\widetilde{E}$ (see (18)), while their signs are opposite:

$$\frac{-i}{\beta L}E_{\rm ext} \,=\, \mu\,\kappa^2\Big[\int f^{\rm b} f^{\rm c}\,{\rm d}^2x \,-\, \kappa^{-2}\oint f^{\rm b}\frac{\partial}{\partial n}f^{\rm c}\,{\rm d}s\Big]\,. \tag{22}$$

It is just the contribution due to $C_i$, which is responsible for the smoothed out representation (22). After all, we redefine $\beta \to \beta^{-1}$, and the leading estimate for $\mathcal{Z}$ acquires, with respect of (18) and (22), the following form:

$$\begin{aligned} &\mathcal{Z} \,\sim\, {\rm const}\times e^{-\beta\mathcal{W}}\,,\\ &\frac{\mathcal{W}}{L} \,\equiv\, -\frac{\mu b_1 b_2}{2\pi}\,\mathcal{U}(\kappa|\mathbf{y}_1-\mathbf{y}_2|)\,, \qquad \mathcal{U}(s)\equiv \log\big(\frac{\gamma}{2}s\big) \,+\, K_0(s)\,. \end{aligned} \tag{23}$$

Equation (23) is valid provided the "electro-neutrality" condition $b_1 + b_2 = 0$ is respected, i.e., the pair of dislocations in question forms the *dislocation dipole.* This condition prevents divergency due to the large logarithm in (21).

Let us calculate the force $F = -\frac{{\rm d}\mathcal{W}}{{\rm d}|\mathbf{y}_{12}|}$. Its expression

$$\frac{F}{L} \,=\, \frac{\mu b_1 b_2 \kappa}{2\pi}\,f(\kappa|\mathbf{y}_{12}|)\,, \qquad f(s) \,\equiv\, \frac{{\rm d}\mathcal{U}}{{\rm d}s} \,=\, s^{-1} \,-\, K_1(s)\,, \tag{24}$$

demonstrates that $\mathcal{W}$ (23) at large separation $|\mathbf{y}_{12}|$ corresponds to the energy of the Coulomb attraction between two point charges of unlike signs ($b_1 b_2 < 0$). The function $f(s)$ is positive and goes to zero like $1/s$ at $s \to \infty$, or like $s\log(A/s)$ at $s \to 0$. The maximum of $f(s)$ (24) occurs at $s \approx 1.1$, i.e., the maximal attraction of two opposite dislocations forming the dipole occurs at $|\mathbf{y}_1 - \mathbf{y}_2| \approx \frac{1.1}{\kappa}$. Effect of so-called *image dislocations* [57], which ensure a free surface boundary condition, is neglected so far in $\mathcal{W}$ (23) [3]. Effects due to rotation of the ends of the cylinder containing the dislocations are neglected also.

Generalization to the case of $\mathcal{N}$ dislocations is straightforward. For instance, the corresponding extremum condition (5) takes the form:

$$\Delta f^{\rm b} \,=\, i\frac{2}{\beta}\,\partial_1 e_2^P \,=\, \frac{-i}{\beta}\rho(\mathbf{x})\,, \qquad \rho(\mathbf{x}) \,\equiv\, \sum_{I=1}^{\mathcal{N}} j(\mathbf{x}-\mathbf{y}_I)\,, \tag{25}$$

where $j(\mathbf{x}-\mathbf{y}_I) \equiv b_I \overset{(2)}{\delta}(\mathbf{x}-\mathbf{y}_I)$, and $\rho(\mathbf{x})$ is thus the dislocation density. Eventually, the effective energy we are interested in, $\mathcal{W} \equiv \frac{-1}{\beta}\log\mathcal{Z}$, takes the form:

$$\mathcal{W} \,=\, 2\mu\int \partial_1 e_2^P(\mathbf{x})\,\big((\Delta-\kappa^2)^{-1} \,-\, \Delta^{-1}\big)\,\partial_1 e_2^P(\mathbf{s})\,{\rm d}^2x\,{\rm d}^2s\,, \tag{26}$$

[3] The free-boundary problem for the stress distribution around a screw dislocation inside the wall of hollow cylinder has been investigated in [21].

where Eq. (25) has been used (here and below the shear modulus is re-scaled: $\mu L \to \mu$). Transforming $\mathcal{W}$ (26) further, we represent it as the "pair" potential dependent on the dislocation positions $\{\mathbf{y}_I\} \equiv \{\mathbf{y}_I\}_{1\le I\le\mathcal{N}}$:

$$
\begin{aligned}
\mathcal{W} &\equiv \mathcal{W}\big(\{\mathbf{y}_I\}\big) = \\
&= \frac{-\mu}{4\pi}\int \rho(\mathbf{x})\,\big(\log|\mathbf{x}-\mathbf{s}| + K_0(\kappa|\mathbf{x}-\mathbf{s}|)\big)\,\rho(\mathbf{s})\,\mathrm{d}^2x\,\mathrm{d}^2s \\
&= \frac{-\mu}{4\pi}\sum_{I\neq J} b_I b_J\,\mathcal{U}(\kappa|\mathbf{y}_I-\mathbf{y}_J|)\,,
\end{aligned}
\tag{27}
$$

where $\mathcal{U}(\cdot)$ is defined by (23), and the "electro-neutrality" condition $\sum_{I=1}^{\mathcal{N}} b_I = 0$ is taken into account. The distances in (27) are referred, for simplicity, to unit lattice spacing of a cubic crystal.

Let us consider thermodynamical ensemble of positive and negative modified screw dislocations located, respectively, at $\{\mathbf{y}_I^+\}_{1\le I\le\mathcal{N}}$ and $\{\mathbf{y}_I^-\}_{1\le I\le\mathcal{N}}$ and possessing unit Burgers vectors $|b_I| = 1$. The corresponding partition function $\mathbf{Z}_C$ can be written as that of electro-neutral plasma of positive and negative charges with modified Coulomb-like coupling:

$$
\begin{aligned}
\mathbf{Z}_C = &\sum_{\mathcal{N}=0}^{\infty}\frac{1}{\mathcal{N}!\,\mathcal{N}!}\prod_{I=1}^{\mathcal{N}}\int \mathrm{d}^2\mathbf{y}_I^+\prod_{J=1}^{\mathcal{N}}\int \mathrm{d}^2\mathbf{y}_J^-\,\exp\Big[-2\beta\mathcal{N}\Lambda + \\
&+\frac{\beta\mu}{4\pi}\Big(\sum_{I\neq J}\mathcal{U}(\kappa|\mathbf{y}_I^+-\mathbf{y}_J^+|) + \sum_{I\neq J}\mathcal{U}(\kappa|\mathbf{y}_I^- -\mathbf{y}_J^-|) - 2\sum_{I\neq J}\mathcal{U}(\kappa|\mathbf{y}_I^+-\mathbf{y}_J^-|)\Big)\Big]\,,
\end{aligned}
\tag{28}
$$

where $2\mathcal{N}$ is the number of charges, and the chemical potential $\Lambda$ (per dislocation) is introduced. The representation (28) implies that the exponentials $e^{-\beta\mathcal{W}}$, where $\mathcal{W}$ corresponds to (27), are summed up with respect of all possible positions of the dislocations inside the cylinder's cross-section (in fact, the summations are replaced by the integrations). The representation (28) generalizes an analogous expression [47] for a system of the world-sheet vortices. In our case the smoothed out potential $\mathcal{U}(s)$ appears self-consistently while an artificially regularized logarithmic potential is used in [47]. It is appropriate to remind that the Coulomb gas of point-like charges is equivalent to the *sine-Gordon* field theory [58–60].

# 3 The correlation functions

## 3.1 Field-theoretical derivation of the stress-stress correlation function

Gaining the experience of the derivation of the partition function of the Coulomb-like plasma (28), let us pass on to investigation of the corresponding correlation functions. The partition function $\mathcal{Z}$ of the field theory presented in Section 2 is taken as a starting point. Define the two-point *stress-stress correlation functions* $\langle\sigma_i^{\#}(\mathbf{x}_1)\,\sigma_j^{\#}(\mathbf{x}_2)\rangle$ (# is either b or c) by means of the following functional averages [37–40]:

$$
\langle\sigma_i^{\#}(\mathbf{x}_1)\,\sigma_j^{\#}(\mathbf{x}_2)\rangle \equiv \frac{1}{\mathcal{Z}}\int \sigma_i^{\#}(\mathbf{x}_1)\,\sigma_j^{\#}(\mathbf{x}_2)\,e^{-\beta W}\mathcal{D}(\sigma_i^{\mathrm{b}},\sigma_i^{\mathrm{c}},u,e_i)\,,
\tag{29}
$$

where $\mathcal{Z}$ is expressed by Eqs. (1), (2), (4). The functional $W$ is written as dependent on the "external" source $\mathcal{P}_i$ ($i = 1, 2$) since the correlators (29) (as well as the partition function itself) are defined with respect of a specific distribution of the dislocations. In other words, specification of $\mathcal{P}_i$ by means of a choice of the plastic source $e_i^P$ is required. Approach of the generating functional [45,46] provides a natural way to evaluate (29) by means of the functional integration [37–39]. We introduce the generating functional $\mathcal{G}[\mathbf{J}^{\rm b}, \mathbf{J}^{\rm c} \,|\, \boldsymbol{\mathcal{P}}]$ as the functional integral dependent on two auxiliary (in principle, unphysical) sources $\mathbf{J}^{\rm b}$, $\mathbf{J}^{\rm c}$, as well as on the source $\boldsymbol{\mathcal{P}}$:

$$\mathcal{G}[\mathbf{J}^{\rm b}, \mathbf{J}^{\rm c} \,|\, \boldsymbol{\mathcal{P}}] \;=\; \int e^{-\beta W + iL\int (J_i^{\rm b}\sigma_i^{\rm b} + J_j^{\rm c}\sigma_j^{\rm c})\,{\rm d}^2x}\, \mathcal{D}(\sigma_i^{\rm b}, \sigma_i^{\rm c}, u, e_i)\,. \tag{30}$$

Now the normalization factor is included into the integration measure, and each bold-faced notation, $\mathbf{J}^{\#}$ ($\#$ is b or c) or $\boldsymbol{\mathcal{P}}$, implies two components, say, $J_1^{\#}$ and $J_2^{\#}$. The source $\boldsymbol{\mathcal{P}}$ is standing separately in left-hand side of (30) since its meaning is different. The correlators we are interested in, $\langle \sigma_i^{\#}(\mathbf{x}_1)\, \sigma_j^{\#}(\mathbf{x}_2)\rangle$, appear as follows:

$$\langle \sigma_i^{\#}(\mathbf{x}_1)\, \sigma_j^{\#}(\mathbf{x}_2)\rangle \;=\; \lim_{\mathbf{J}^{\rm b},\, \mathbf{J}^{\rm c}\to 0} \left( \mathcal{G}^{-1}[\mathbf{J}^{\rm b}, \mathbf{J}^{\rm c} \,|\, \boldsymbol{\mathcal{P}}^{\rm ph}]\, \frac{(-i)^2\, \delta^2}{\delta J_i^{\#}(\mathbf{x}_1) \delta J_j^{\#}(\mathbf{x}_2)}\, \mathcal{G}[\mathbf{J}^{\rm b}, \mathbf{J}^{\rm c} \,|\, \boldsymbol{\mathcal{P}}^{\rm ph}] \right). \tag{31}$$

Equation (31) implies that the source $\boldsymbol{\mathcal{P}}$ is replaced by the source $\boldsymbol{\mathcal{P}}^{\rm ph}$ corresponding to a specific choice of the dislocation distribution.

It has to be stressed that the contribution $\propto \int \sigma_i^{\rm b} \mathcal{P}_i\, {\rm d}^2x$ in $E_{\rm ext}$ (4) looks similar to the source term $\propto \int \sigma_i^{\rm b} J_i^{\rm b}\, {\rm d}^2x$ in the exponent of (30). Therefore the variational differentiation with respect of $J_i^{\rm b}$ ($J_i^{\rm b} \to 0$, afterwards) is equivalent to that with respect of $\mathcal{P}_i$, being considered, for an instant, as arbitrary function. Clearly, the source $\mathcal{P}_i$ must take its physical value (as explained above) after the differentiation. Therefore it is appropriate to put $\mathcal{G}[\mathbf{J}^{\rm b}, \mathbf{J}^{\rm c} \,|\, \boldsymbol{\mathcal{P}}]$ (30) as dependent on three arguments: the field theory in question is governed by the physical external source $\mathcal{P}_i$ (related to an actual distribution of the dislocations), while two unphysical ones, $J_i^{\rm b}$ and $J_i^{\rm c}$, enable to derive the correlator.

We shall calculate the stress-stress correlation function $\langle \sigma_i^{\rm tot}(\mathbf{x}_1)\, \sigma_j^{\rm tot}(\mathbf{x}_2)\rangle$ of the physical stress field $\sigma_i^{\rm tot}(\mathbf{x}) \equiv \frac{\beta}{i}(\sigma_i^{\rm b}(\mathbf{x}) + \sigma_i^{\rm c}(\mathbf{x}))$. First, we calculate the generating functional (30) shifting the integration variables so to cancel the terms linear in $\mathbf{J}^{\rm b}$, $\mathbf{J}^{\rm c}$ in the exponent (see Appendix). The result looks as follows:

$$\mathcal{G}[\mathbf{J}, \mathbf{J} \,|\, \boldsymbol{\mathcal{P}}^{\rm ph}] \;=\; e^{-\frac{\mu\beta}{2} Q}\,, \tag{32}$$

where

$$\begin{aligned} Q &\equiv \int \left( \partial_i \mathcal{J}_i \Big( \frac{1}{\Delta} \,-\, \frac{1}{\Delta - \kappa^2} \Big) \partial_k \mathcal{J}_k \,-\, \mathcal{J}_i \frac{\kappa^2}{\Delta - \kappa^2} \mathcal{J}_i \,+\, \Delta J_i \frac{1}{\Delta - \kappa^2} J_i \right) {\rm d}^2x\,, \\ \mathcal{J}_i &\equiv J_i - 2e_i^P \end{aligned} \tag{33}$$

(the "inverses" $\Delta^{-1}$, $(\Delta - \kappa^2)^{-1}$ act as the integral operators). The generating functional (32), (33) is expressed in terms of a single source $J_i(\mathbf{x}) = J_i^{\rm b}(\mathbf{x}) = J_i^{\rm c}(\mathbf{x})$. Then the physical correlation function appears as follows:

$$\langle \sigma_i^{\rm tot}(\mathbf{x}_1) \sigma_j^{\rm tot}(\mathbf{x}_2)\rangle \;=\; \Big(\frac{\beta}{i}\Big)^2 \lim_{\mathbf{J}\to 0} \left( \mathcal{G}^{-1}[\mathbf{J}, \mathbf{J} \,|\, \boldsymbol{\mathcal{P}}^{\rm ph}]\, \frac{(-i)^2\, \delta^2}{\delta J_i(\mathbf{x}_1) \delta J_j(\mathbf{x}_2)}\, \mathcal{G}[\mathbf{J}, \mathbf{J} \,|\, \boldsymbol{\mathcal{P}}^{\rm ph}] \right). \tag{34}$$

We calculate (34) using (32), (33), and obtain the following expression:

$$\langle\sigma_i^{\rm tot}(\mathbf{x}_1)\sigma_j^{\rm tot}(\mathbf{x}_2)\rangle \;=\; \frac{\mu^2}{4}\, e^{-\beta\mathcal{W}} \times \lim_{\mathbf{J}\to 0}\Big[\big(\delta_{J_i(\mathbf{x}_1)}Q\big)\big(\delta_{J_j(\mathbf{x}_2)}Q\big) \;-\; \frac{2}{\mu\beta}\,\delta_{J_i(\mathbf{x}_1)}\delta_{J_j(\mathbf{x}_2)}Q\Big]\,, \tag{35}$$

where $\delta_{J_i(\mathbf{x})} \equiv \delta/\delta J_i(\mathbf{x})$, and $\mathcal{W}$, $Q$ are given by (27), (33). Equation (35) is re-expressed after calculation of the variational derivatives:

$$\begin{aligned}\langle\sigma_i^{\rm tot}(\mathbf{x}_1)\sigma_j^{\rm tot}(\mathbf{x}_2)\rangle \;=\; e^{-\beta\mathcal{W}} \times \Big[\sigma_i^{\rm tot}(\mathbf{x}_1)\sigma_j^{\rm tot}(\mathbf{x}_2) - \\ - \frac{\mu}{2\pi\beta}\partial_{(\mathbf{x}_1)_i}\partial_{(\mathbf{x}_2)_j}\mathcal{U}(\kappa|\mathbf{x}_1-\mathbf{x}_2|)\Big]\,,\end{aligned} \tag{36}$$

where

$$\sigma_i^{\rm tot}(\mathbf{x}) \;=\; \frac{\mu}{\pi}\epsilon_{ik}\,\partial_{(\mathbf{x})_k}\int \mathcal{U}(\kappa|\mathbf{x}-\mathbf{s}|)\,\partial_1 e_2^P(\mathbf{s})\mathrm{d}\mathbf{s} \tag{37}$$

is the total elastic stress of the dislocational configuration. The first term inside the square brackets is just due to the plastic strain considered as the physical external source. The exponential factor in (36) is the Boltzmann weight containing in its exponent the energy of the ensemble of the dislocations.

Consider, for a comparison, our theory without the influence of the core energy, i.e., at $\ell = 0$. Derive, firstly, the stress-stress correlator $\langle\sigma_i^{\rm b}(\mathbf{x}_1)\sigma_j^{\rm b}(\mathbf{x}_2)\rangle$ using $e_i^P$ as the unphysical source that becomes zero after the variation:

$$\langle\sigma_i^{\rm b}(\mathbf{x}_1)\sigma_j^{\rm b}(\mathbf{x}_2)\rangle \;=\; \frac{-\mu}{2\pi\beta}\,\partial_{(\mathbf{x}_1)_i}\partial_{(\mathbf{x}_2)_j}\log|\mathbf{x}_1-\mathbf{x}_2|\,. \tag{38}$$

The plastic field, as the source of a specific distribution of the dislocations, is responsible for the second term in the square brackets in (35). Let the plastic source be the physical one respecting Eq. (25). Then we obtain:

$$\begin{aligned}\langle\sigma_i^{\rm b}(\mathbf{x}_1)\sigma_j^{\rm b}(\mathbf{x}_2)\rangle \;=\; e^{-\beta\mathcal{W}} \times \Big[\frac{-\mu}{2\pi\beta}\partial_{(\mathbf{x}_1)_i}\partial_{(\mathbf{x}_2)_j}\log|\mathbf{x}_1-\mathbf{x}_2| \\ + \frac{\mu^2}{4\pi^2}\sum_{I,J} b_I b_J\big(\epsilon_{ik}\partial_{(\mathbf{x}_1)_k}\log|\mathbf{x}_1-\mathbf{y}_I|\big)\big(\epsilon_{jl}\partial_{(\mathbf{x}_2)_l}\log|\mathbf{x}_2-\mathbf{y}_J|\big)\Big]\,,\end{aligned} \tag{39}$$

where $\mathcal{W}$ is given by (27) although with $\mathcal{U}$ replaced appropriately by the logarithm.

The representation (36) corresponds to a specific spatial distribution of collection of the dislocations. In the sequel we shall average the correlator $\langle\sigma_i^{\rm b}(\mathbf{x}_1)\sigma_j^{\rm b}(\mathbf{x}_2)\rangle$ over possible positions of the dislocations.

## 3.2 Mean square of the dipole momentum

We shall investigate the thermodynamical ensemble of the dislocations using so-called *dipole phase* approximation which implies that pairs of the dislocations with opposite signs (located in $\mathbf{x}_I^{\pm}$, $1 \le I \le \mathcal{N}$) are bound into "molecules". The corresponding partition function is specialized in the form different from (28):

$$\begin{aligned}\mathbf{Z}_{\rm dip} \;=\; \sum_{\mathcal{N}=0}^{\infty}\frac{1}{\mathcal{N}!}\prod_{I=1}^{\mathcal{N}}\int \mathrm{d}^2\boldsymbol{\xi}_I\int \mathrm{d}^2\boldsymbol{\eta}_I\,\exp\Big[-2\beta\mathcal{N}\Lambda- \\ -\beta\Big(\sum_{I=1}^{\mathcal{N}} w(\boldsymbol{\eta}_I) \;+\; \sum_{I\neq J} w_{IJ}\Big)\Big]\,,\end{aligned} \tag{40}$$

where $w(\boldsymbol{\eta}_I)$ is the energy of $I^{\mathrm{th}}$ dipole centered in $\boldsymbol{\xi}_I = (\mathbf{x}_I^+ + \mathbf{x}_I^-)/2$ with the dipole momentum $\boldsymbol{\eta}_I = \mathbf{x}_I^+ - \mathbf{x}_I^-$, while $w_{IJ}$ is the energy of interaction between $I^{\mathrm{th}}$ and $J^{\mathrm{th}}$ dipoles [47].

First of all, let us calculate a mean square of the dipole momentum for a single molecule:

$$\langle \boldsymbol{\eta}^2 \rangle = \frac{\displaystyle\int \exp(-\beta w(\boldsymbol{\eta}))\, \boldsymbol{\eta}^2 \mathrm{d}\boldsymbol{\eta}}{\displaystyle\int \exp(-\beta w(\boldsymbol{\eta}))\, \mathrm{d}\boldsymbol{\eta}} . \tag{41}$$

The average $\langle \boldsymbol{\eta}^2 \rangle$ (41) has been calculated in [3] for two-dimensional gas of particles with charges $\pm q$ interacting through the potential looking as follows:

$$\begin{array}{rl} 2\Lambda - 2q_I\, q_J \mathcal{U}(|\mathbf{x}_I - \mathbf{x}_J|)\,, & |\mathbf{x}_I - \mathbf{x}_J| > a\,, \\ 0\,, & |\mathbf{x}_I - \mathbf{x}_J| < a\,, \end{array}$$

where $\mathcal{U}(|\mathbf{x}_I - \mathbf{x}_J|) \equiv \log \frac{|\mathbf{x}_I - \mathbf{x}_J|}{a}$, $\mathbf{x}_I$ is the $I^{\mathrm{th}}$ charge position, and $a$ is an appropriate cutoff (e.g., the particle diameter, or lattice spacing). Besides, $2\Lambda$ is the energy necessary to create a pair of opposite charges at the distance $a$, while the number of particles is constrained by overall electrical neutrality. The dipole energy is given by $\beta w(\boldsymbol{\eta}) = \mathcal{K}\mathcal{U}(|\boldsymbol{\eta}|)$, where $\mathcal{K} = 2\beta q^2$, and the average (41) takes the form [3]:

$$\langle \boldsymbol{\eta}^2 \rangle = a^2 \frac{\mathcal{K} - 2}{\mathcal{K} - 4} = a^2 \frac{\beta q^2 - 1}{\beta q^2 - 2}\,, \tag{42}$$

where it is assumed that $\beta q^2 > 2$, and the lower integration boundary is $a$. Therefore, $\langle \boldsymbol{\eta}^2 \rangle \approx a^2$ in the limit of zero temperature. The average (42) infinitely grows at $T$ near the critical temperature $T_c$ given by $\beta_c q^2 = 2$.

The two-particle potential considered in [47] is expressed as $\beta w(\boldsymbol{\eta}) = 2\pi\mathcal{K}\mathcal{U}(|\boldsymbol{\eta}|)$, where $\beta$ is an effective parameter viewed as inverse temperature, $\mathcal{K} = 2\beta q^2$, and $\mathcal{U}(|\boldsymbol{\eta}|)$ is regularized at small momenta, $\mathcal{U}(|\boldsymbol{\eta}|) = \frac{1}{2} \log \frac{a^2 + |\boldsymbol{\eta}|^2}{a^2}$. Then, Eq. (41) gives the answer at $\mathcal{K} > 2/\pi$:

$$\langle \boldsymbol{\eta}^2 \rangle = a^2 \frac{1}{\pi\mathcal{K} - 2}\,, \tag{43}$$

i.e., the dipole momentum of a single molecule is not too large provided the temperature is decreased. It can be verified that $\langle \boldsymbol{\eta}^2 \rangle$ (42) is strictly greater than $\langle \boldsymbol{\eta}^2 \rangle$ (43) at $\mathcal{K} > 4$, i.e., in the second case the molecules are more compact at small enough temperatures.

The present paper deals with the dipole energy $\mathcal{U}(\kappa|\boldsymbol{\eta}|)$ (23), and the average (41) is specified as follows:

$$\kappa^2 \langle \boldsymbol{\eta}^2 \rangle = \frac{\displaystyle\int_0^\infty \exp(-\mathcal{K}(\log \eta + K_0(\eta)))\, \eta^3\, \mathrm{d}\eta}{\displaystyle\int_0^\infty \exp(-\mathcal{K}(\log \eta + K_0(\eta)))\, \eta\, \mathrm{d}\eta}\,, \tag{44}$$

where $\mathcal{K} = \mu b^2 \beta / 2\pi$. The integral in the nominator of (44) diverges at $\mathcal{K} < 4$. Since dissociation is most probable for pairs of the dislocations with $|b| = 1$, the dipolar phase does not exist at the temperature $T > T_c \equiv \frac{\mu}{8\pi}$.

Remind that estimates for the radius of the dislocation core $r_c$ have been proposed in [29, 31, 33] in the form $r_c \simeq \eta_b/\kappa$, where $\eta_b = 4.0$ [29], $\eta_b = 6.0$ [33], or $\eta_b = 10.0$ [31].

In turn, the estimates for $\kappa^{-1}$ in terms of interatomic spacing $a$ have been obtained in the form: $\kappa^{-1} \approx 0.39\, a$ [28], $\kappa^{-1} \approx 0.399\, a$ [33], $\kappa^{-1} \approx 0.25\, a$ [29]. For instance, $r_c \approx 1.5a$ according to [29], while $r_c \approx 2.4a$ according to [33].

To estimate (44), it is appropriate to split each integration into two parts: from $\eta = 0$ to $\eta = \eta_b$ and from $\eta = \eta_b$ to infinity, so that $K_0(\eta)$ is neglected above $\eta_b$ with enough accuracy. Therefore, we estimate (44) at $\mathcal{K}$ close to its "critical" value, $\mathcal{K} \searrow 4$:

$$\langle \boldsymbol{\eta}^2 \rangle \simeq \frac{2\eta_b^2}{\kappa^2(1 + 2\eta_b^2 \mathsf{A}^{-1})} \frac{1}{\mathcal{K} - 4}, \qquad \mathsf{A}^{-1} \equiv \int_0^{\eta_b} \exp(-4(\log \eta + K_0(\eta)))\, \eta \, \mathrm{d}\eta . \tag{45}$$

For instance, Eq. (45) looks approximately at $\eta_b \gtrsim 6.0$:

$$\langle \boldsymbol{\eta}^2 \rangle \simeq \frac{\mathsf{A}}{\kappa^2} \frac{1}{\mathcal{K} - 4}, \quad \mathsf{A} \approx 2.5 , \tag{46}$$

where $\kappa^{-2}$ can be taken according either to [29] or [33]. In both cases, (46) corresponds to more compact dipoles in comparison with (43).

Double-sided estimate can be obtained for the potential $\mathcal{U}(\kappa|\boldsymbol{\eta}|)$ (23) by adjusting appropriate trial functions thus resulting in a double-sided estimate for $\langle \boldsymbol{\eta}^2 \rangle$ (44) valid at $\mathcal{K}$ large enough:

$$\frac{1}{\mathcal{K}^2} < \kappa^2 \langle \boldsymbol{\eta}^2 \rangle < \frac{1}{\mathcal{K}} , \tag{47}$$

where $\kappa^{-1}$ can be chosen according to [28], [29], or [33]. Equation (47) implies that $\langle \boldsymbol{\eta}^2 \rangle$ tends to zero faster in comparison with the rule (43). This is just due to the dipole energy profile (23) used instead of the regularization adopted in [47]. Respectively, the density of the molecules grows at vanishing temperature faster in framework of the present approach.

## 3.3 The correlator of two stresses

We continue to consider the dipole phase in the approximation of non-interacting dipoles. Let us turn to the stress-stress correlation function $\langle \sigma_i^{\text{tot}}(\mathbf{x}_1)\, \sigma_j^{\text{tot}}(\mathbf{x}_2) \rangle$ given by Eqs. (36), (37) and average it over positions of the dislocation dipoles. To this end we shall follow [47] where contributions due to the vortex dipoles into the asymptotical behavior of appropriate correlation functions of the string models have been investigated. We shall denote the new average as $\langle\langle \sigma_i^{\text{tot}}(\mathbf{x}_1)\, \sigma_j^{\text{tot}}(\mathbf{x}_2) \rangle\rangle$, and its expression arises as follows:

$$\begin{aligned} \langle\langle \sigma_i^{\text{tot}}(\mathbf{x}_1)\, \sigma_j^{\text{tot}}(\mathbf{x}_2) \rangle\rangle &= \frac{-\mu}{2\pi\beta} \partial_{(\mathbf{x}_1)_i} \partial_{(\mathbf{x}_2)_j} \mathcal{U}(\kappa|\mathbf{x}_1 - \mathbf{x}_2|) \\ &+ \mathbf{Z}_{\text{dip}}^{-1} \sum_{\substack{\text{number of dipoles,} \\ \text{dipoles positions}}} \sigma_i^{\text{tot}}(\mathbf{x}_1) \sigma_j^{\text{tot}}(\mathbf{x}_2)\, e^{-\beta \mathcal{W}} , \end{aligned} \tag{48}$$

where $\mathbf{Z}_{\text{dip}}$ is the partition function (40).

According to (47), the dipoles are very compact since the dipole momenta are not too large at small enough temperature: $\langle \boldsymbol{\eta}^2 \rangle \ll \kappa^{-2}$. Therefore summation over the dipole positions can be replaced by integration [47]. We use the dipole's center of mass and momentum coordinates, respectively, $\boldsymbol{\xi}_L = (\mathbf{y}_L^+ + \mathbf{y}_L^-)/2$ and $\boldsymbol{\eta}_L = \mathbf{y}_L^+ - \mathbf{y}_L^-$ for each pair of opposite dislocations at $\mathbf{y}_L^{\pm}$ forming $L^{\rm th}$ dipole ($1 \le L \le \mathcal{N}$). Therefore the sum in right-hand side of (48) takes the form:

$$
\begin{aligned}
&\sum_{\text{numbers , positions}} \sigma_i^{\rm tot}(\mathbf{x}_1)\sigma_j^{\rm tot}(\mathbf{x}_2)\, e^{-\beta\mathcal{W}} \;= \\
&= \Big(\frac{\mu b}{2\pi}\Big)^2 \epsilon_{ik}\epsilon_{jl}\, \partial_{(\mathbf{x}_1)_k}\partial_{(\mathbf{x}_2)_l} \sum_{\mathcal{N}=1}^{\infty} \frac{1}{\mathcal{N}!}\prod_{I=1}^{\mathcal{N}} \int {\rm d}^2\boldsymbol{\xi}_I \int {\rm d}^2\boldsymbol{\eta}_I\, \exp\!\big(-\beta(2\Lambda \,+\, w(\boldsymbol{\eta}_I))\big) \\
&\times \sum_{K,L=1}^{\mathcal{N}} \big[\mathcal{U}(\kappa|\mathbf{x}_1 - \mathbf{y}_K^{+}|) \,-\, \mathcal{U}(\kappa|\mathbf{x}_1 - \mathbf{y}_K^{-}|)\big] \\
&\qquad\qquad \times \big[\mathcal{U}(\kappa|\mathbf{x}_2 - \mathbf{y}_L^{+}|) \,-\, \mathcal{U}(\kappa|\mathbf{x}_2 - \mathbf{y}_L^{-}|)\big]\,,
\end{aligned}
\tag{49}
$$

where $\mathcal{N}$ is the number of dipoles, and the representation (37) is used for $\sigma_i^{\rm tot}(\mathbf{x})$. We use the estimate $|\boldsymbol{\eta}_L| \ll |\mathbf{x} - \boldsymbol{\xi}_L|$ (compactness of the dipoles) and adopt in leading approximation [47]:

$$
\mathcal{U}(\kappa|\mathbf{x} - \mathbf{y}_L^{+}|) \,-\, \mathcal{U}(\kappa|\mathbf{x} - \mathbf{y}_L^{-}|) \,\approx\, -\,(\boldsymbol{\eta}_L, \partial_{\mathbf{x}})\,\mathcal{U}(\kappa|\mathbf{x} - \boldsymbol{\xi}_L|)\,, \tag{50}
$$

where the notation $(\cdot,\cdot)$ for the scalar product of 2-vectors is introduced. The relation (50) allows to re-express (49) as follows:

$$
\begin{aligned}
&\Big(\frac{\mu b}{2\pi}\Big)^2 \epsilon_{ik}\epsilon_{jl}\, \partial_{(\mathbf{x}_1)_k}\partial_{(\mathbf{x}_2)_l} \sum_{\mathcal{N}=1}^{\infty} \frac{1}{\mathcal{N}!}\prod_{I=1}^{\mathcal{N}} \int {\rm d}^2\boldsymbol{\xi}_I \int {\rm d}^2\boldsymbol{\eta}_I\, \exp\!\big(-\beta(2\Lambda \,+\, w(\boldsymbol{\eta}_I))\big) \\
&\qquad \times \sum_{L=1}^{\mathcal{N}} (\boldsymbol{\eta}_L, \partial_{\mathbf{x}_1})\,\mathcal{U}(\kappa|\mathbf{x}_1 - \boldsymbol{\xi}_L|)\,(\boldsymbol{\eta}_L, \partial_{\mathbf{x}_2})\,\mathcal{U}(\kappa|\mathbf{x}_2 - \boldsymbol{\xi}_L|)\,.
\end{aligned}
\tag{51}
$$

To proceed with (51), essential technical task is to calculate the integral:

$$
\begin{aligned}
&\int {\rm d}^2\boldsymbol{\xi} \int {\rm d}^2\boldsymbol{\eta}\, \exp\!\big(-\beta(2\Lambda \,+\, w(\boldsymbol{\eta}))\big) \\
&\times (\boldsymbol{\eta}, \partial_{\mathbf{x}_1})(\boldsymbol{\eta}, \partial_{\mathbf{x}_2})\mathcal{U}(\kappa|\mathbf{x}_1 - \boldsymbol{\xi}|)\,\mathcal{U}(\kappa|\mathbf{x}_2 - \boldsymbol{\xi}|)\,.
\end{aligned}
\tag{52}
$$

First, we express the $\boldsymbol{\eta}$-integration by means of the relation

$$
\frac{\displaystyle\int \exp\!\big(-2\beta\Lambda - \mathcal{K}(\log(\frac{\gamma}{2}\kappa\eta) + K_0(\kappa\eta))\big)\,\eta_i\eta_j\, {\rm d}^2\boldsymbol{\eta}}{\displaystyle\int \exp\!\big(-2\beta\Lambda - \mathcal{K}(\log(\frac{\gamma}{2}\kappa\eta) + K_0(\kappa\eta))\big)\, {\rm d}^2\boldsymbol{\eta}} \;=\; \frac{\delta_{ij}}{2}\langle\boldsymbol{\eta}^2\rangle\,, \tag{53}
$$

where $\mathcal{K} = \frac{\mu b^2\beta}{2\pi}$, $\eta = |\boldsymbol{\eta}|$, and $\langle\boldsymbol{\eta}^2\rangle$ is given by (44). Then, after introducing the notation $\bar{N}$ for the dipole density [3, 47]:

$$
\bar{N} \,\equiv\, \int \exp\!\big(-2\beta\Lambda - \mathcal{K}(\log(\frac{\gamma}{2}\kappa\eta) + K_0(\kappa\eta))\big)\, {\rm d}^2\boldsymbol{\eta}\,, \tag{54}
$$

the relation (53) allows to re-express the integral (52) as follows:

$$
\frac{\bar{N}\langle\boldsymbol{\eta}^2\rangle}{2} \int \big(\partial_{\mathbf{x}_1}\mathcal{U}(\kappa|\mathbf{x}_1 - \boldsymbol{\xi}|)\,,\partial_{\mathbf{x}_2}\mathcal{U}(\kappa|\mathbf{x}_2 - \boldsymbol{\xi}|)\big)\, {\rm d}^2\boldsymbol{\xi}\,. \tag{55}
$$

The Green theorem enables to carry out the $\boldsymbol{\xi}$-integration in (55). Eventually, we use the partition function $\mathbf{Z}_{\rm dip}$ (40) and obtain:

$$\begin{aligned} &\langle\!\langle \sigma^{\rm tot}_i(\mathbf{x}_1)\,\sigma^{\rm tot}_j(\mathbf{x}_2)\rangle\!\rangle \;=\; \frac{-\mu}{2\pi\beta}\,\partial_{(\mathbf{x}_1)_i}\partial_{(\mathbf{x}_2)_j}\mathcal{U}(\kappa|\Delta\mathbf{x}|) \\ &-\bar{N}\langle\boldsymbol{\eta}^2\rangle\,\frac{\mu^2b^2}{4\pi}\,\epsilon_{ik}\epsilon_{jl}\,\partial_{(\mathbf{x}_1)_k}\partial_{(\mathbf{x}_2)_l}\big(\log|\Delta\mathbf{x}|\;+\;K_0(\kappa|\Delta\mathbf{x}|)+\frac{\kappa|\Delta\mathbf{x}|}{2}\,K_1(\kappa|\Delta\mathbf{x}|)\big)\,, \end{aligned} \tag{56}$$

where (as well as below) $\Delta\mathbf{x}\equiv\mathbf{x}_1-\mathbf{x}_2$.

At large separation of the arguments, $|\mathbf{x}_1-\mathbf{x}_2|\gg\kappa^{-1}$, the asymptotic of (56) is governed by the logarithmic contribution since the modified Bessel functions decay exponentially:

$$\begin{aligned} &\langle\!\langle \sigma^{\rm tot}_i(\mathbf{x}_1)\,\sigma^{\rm tot}_j(\mathbf{x}_2)\rangle\!\rangle \;\simeq\; \frac{-\mu}{2\pi\beta}\,\partial_{(\mathbf{x}_1)_i}\partial_{(\mathbf{x}_2)_j}\log|\Delta\mathbf{x}| \\ &-\bar{N}\langle\boldsymbol{\eta}^2\rangle\,\frac{\mu^2b^2}{4\pi}\,\epsilon_{ik}\epsilon_{jl}\,\partial_{(\mathbf{x}_1)_k}\partial_{(\mathbf{x}_2)_l}\log|\Delta\mathbf{x}|\;= \\ &=\Big(\frac{-\mu}{2\pi\beta}\;+\;\bar{N}\langle\boldsymbol{\eta}^2\rangle\,\frac{\mu^2b^2}{4\pi}\Big)\,\partial_{(\mathbf{x}_1)_i}\partial_{(\mathbf{x}_2)_j}\log|\Delta\mathbf{x}|\;+\;\bar{N}\langle\boldsymbol{\eta}^2\rangle\,\frac{\mu^2b^2}{2}\delta_{ij}\,\overset{(2)}{\delta}(\mathbf{x}_1-\mathbf{x}_2)\,, \end{aligned} \tag{57}$$

where the relation $\epsilon_{ik}\epsilon_{jl}=\delta_{ij}\delta_{kl}-\delta_{il}\delta_{kj}$ is taken into account. Besides, the $\delta$-like term in right-hand side of (57) is due to the following rule of differentiation of the logarithm:

$$\begin{aligned} &\partial_{(\mathbf{x}_1)_k}\partial_{(\mathbf{x}_2)_l}\log|\mathbf{x}_1-\mathbf{x}_2|\;= \\ &=\;\frac{1}{|\mathbf{x}_1-\mathbf{x}_2|^2}\Big(-\delta_{kl}\;+\;2\frac{(\mathbf{x}_1-\mathbf{x}_2)_k\,(\mathbf{x}_1-\mathbf{x}_2)_l}{|\mathbf{x}_1-\mathbf{x}_2|^2}\Big)\;-\;\pi\,\delta_{kl}\,\overset{(2)}{\delta}(\mathbf{x}_1-\mathbf{x}_2)\,. \end{aligned} \tag{58}$$

The $\delta$-term in right-hand side of (57) is irrelevant for the asymptotical behavior of the correlation function. Therefore the stress-stress correlator (being considered with dislocations as well as without them) decreases as $|\mathbf{x}_1-\mathbf{x}_2|^{-2}$ at growing separation $|\mathbf{x}_1-\mathbf{x}_2|$. However the $\delta$-term is crucial for expression of the shear modulus by means of the stress-stress correlation functions integrated over their spatial arguments (see the next Section).

The asymptotical law $|\mathbf{x}_1-\mathbf{x}_2|^{-2}$ is due to the analytical structure of the logarithm differentiated. This law being extrapolated to small distances $|\mathbf{x}_1-\mathbf{x}_2|\ll 1$ would imply a singular behavior of the stress-stress correlator in question. In the present approach, the short-distance behavior of the correlation function is less singular due to the core influence. First, we obtain the following asymptotics at $|\mathbf{x}_1-\mathbf{x}_2|\ll\kappa^{-1}$:

$$\begin{aligned} &\frac{-\mu}{2\pi\beta}\,\partial_{(\mathbf{x}_1)_i}\partial_{(\mathbf{x}_2)_j}\mathcal{U}(\kappa|\mathbf{x}_1-\mathbf{x}_2|)\;\simeq \\ &\simeq\;\frac{-\mu}{2\pi\beta}\,\frac{\kappa^2}{2}\Big[\delta_{ij}\,\Big(-\frac{1}{2}\;+\;\log\big(\frac{\gamma}{2}\kappa|\Delta\mathbf{x}|\big)\Big)\;+\;\frac{(\mathbf{x}_1-\mathbf{x}_2)_i\,(\mathbf{x}_1-\mathbf{x}_2)_j}{|\mathbf{x}_1-\mathbf{x}_2|^2} \\ &+\mathcal{O}(|\Delta\mathbf{x}|^2\log|\Delta\mathbf{x}|)\Big]\,. \end{aligned} \tag{59}$$

Since purely logarithmic contribution is canceled in the potential $\mathcal{U}$, the estimate (59) demonstrates only the logarithmic divergency instead of the inverse square law. Further, the remaining part of (56) gives the contribution:

$$\bar{N}\langle\boldsymbol{\eta}^2\rangle\,\frac{\mu^2b^2\kappa^2}{16\pi}\,\big(\delta_{ij}\;+\;\mathcal{O}(|\Delta\mathbf{x}|^2\log|\Delta\mathbf{x}|)\big)\,, \tag{60}$$

and the final result looks as follows:

$$\begin{aligned}\langle\!\langle \sigma_i^{\rm tot}(\mathbf{x}_1)\,\sigma_j^{\rm tot}(\mathbf{x}_2)\rangle\!\rangle \;\simeq\; \frac{-\mu}{2\pi\beta}\,\frac{\kappa^2}{2}\Big[\delta_{ij}\,\Big(-\frac{1}{2}\;-\;\bar{N}\langle\boldsymbol{\eta}^2\rangle\,\frac{\mu b^2\beta}{4}\;+\;\log\big(\frac{\gamma}{2}\kappa|\Delta\mathbf{x}|\big)\Big)\\ +\,\frac{(\mathbf{x}_1-\mathbf{x}_2)_i\,(\mathbf{x}_1-\mathbf{x}_2)_j}{|\mathbf{x}_1-\mathbf{x}_2|^2}\;+\;\mathcal{O}(|\Delta\mathbf{x}|^2\log|\Delta\mathbf{x}|)\Big]\,.\end{aligned} \tag{61}$$

We considered the approximation of non-interacting dipoles. When dipoles are close each other, the energy of dipole-dipole interaction becomes important. Interaction between different dipoles can also be taken into account in the present framework. Moreover, for sufficiently dense gas of dipoles second order corrections to the stress fields inside the core could become important [36]. However, this should be a subject of separate investigation.

# 4 The renormalization of the shear modulus

The present section is to investigate the *renormalization* of the shear modulus caused by the presence of the modified screw dislocations. To this end we shall use the stress-stress correlator obtained. One should refer to the original paper [9] for the definition of inverse of the tensor of renormalized elastic constants in terms of appropriate correlation function in presence of dislocations. Further details on the dislocation contribution to the elastic constants can be found in [9] and [16] (devoted, respectively, to two- and three-dimensional situations). Adopting the corresponding definitions [9, 16], we shall consider the following expression for the renormalized shear modulus $\mu_{\rm ren}$:

$$\frac{1}{\mu_{\rm ren}}\;\equiv\;\frac{\beta}{\mu^2\mathcal{S}}\sum_{i,k=1,2}\iint\langle\!\langle \sigma_i^{\rm tot}(\mathbf{x}_1)\,\sigma_k^{\rm tot}(\mathbf{x}_2)\rangle\!\rangle\;{\rm d}^2\mathbf{x}_1{\rm d}^2\mathbf{x}_2\,, \tag{62}$$

where the correlator is defined by (48), $\mathcal{S}$ is the area of the sample's cross-section, and the values of $\mu$, $\mu_{\rm ren}$ are taken in the re-scaled form (see (26), (27)). We use (56) and obtain:

$$\begin{aligned}\sum_{k=1,2}\langle\!\langle \sigma_k^{\rm tot}(\mathbf{x}_1)\,\sigma_k^{\rm tot}(\mathbf{x}_2)\rangle\!\rangle \;=\; \frac{\mu\kappa^2}{2\pi\beta}\Big(K_0(\kappa|\Delta\mathbf{x}|)\,+\\ +\,\bar{N}\langle\boldsymbol{\eta}^2\rangle\,\frac{\beta b^2\mu\kappa}{4}\,|\Delta\mathbf{x}|\,K_1(\kappa|\Delta\mathbf{x}|)\Big)\,.\end{aligned} \tag{63}$$

"Non-diagonal" correlators $\langle\!\langle \sigma_k^{\rm tot}(\mathbf{x}_1)\,\sigma_l^{\rm tot}(\mathbf{x}_2)\rangle\!\rangle$, $k \neq l$, are negligible with respect of the two integrations in (62). Therefore one obtains from (62), (63) the following answer:

$$\frac{1}{\mu_{\rm ren}}\;=\;\frac{1}{\mu}\,\mathcal{C}_1(\kappa R)\;+\;\alpha\,\mathcal{C}_2(\kappa R)\,,\qquad \alpha\equiv\bar{N}\langle\boldsymbol{\eta}^2\rangle\,\frac{\beta b^2}{2}\,, \tag{64}$$

where the functions $\mathcal{C}_1(\kappa R)$ and $\mathcal{C}_2(\kappa R)$ are given by the modified Bessel functions:

$$\begin{aligned}\mathcal{C}_1(\kappa R)\;&\equiv\;\frac{\kappa^2}{2\pi\mathcal{S}}\iint K_0(\kappa|\Delta\mathbf{x}|)\,{\rm d}^2\mathbf{x}_1{\rm d}^2\mathbf{x}_2\;=\;1\;-\;2K_1(\kappa R)I_1(\kappa R)\,,\\ \mathcal{C}_2(\kappa R)\;&\equiv\;\frac{\kappa^3}{4\pi\mathcal{S}}\iint K_1(\kappa|\Delta\mathbf{x}|)\,|\Delta\mathbf{x}|\,{\rm d}^2\mathbf{x}_1{\rm d}^2\mathbf{x}_2\\ &=\;2\;-\;2I_1(\kappa R)\big(K_1(\kappa R)\;-\;\kappa R\,K_1'(\kappa R)\big)\,,\end{aligned} \tag{65}$$

where $K_1'(z) = \frac{\mathrm{d}}{\mathrm{d}z} K_1(z)$. The parameter $\alpha$ (64) is proportional to mean area covered by the dipoles, $2\pi\langle\boldsymbol{\eta}^2\rangle\bar{N}$. The renormalization rule (64) demonstrates the dependence of the shear modulus $\mu_{\rm ren}$ on the dimensionless parameter $\kappa R$. The coefficients $\mathcal{C}_1(\kappa R)$ and $\mathcal{C}_2(\kappa R)$ both are positive and less than unity though tend to unity at $\kappa R \to \infty$. We obtain the estimates for $\mathcal{C}_1(\kappa R)$, $\mathcal{C}_2(\kappa R)$ at increasing $\kappa R$:

$$\mathcal{C}_1(\kappa R) \approx 1 - \frac{1}{\kappa R} + \ldots\,, \qquad \mathcal{C}_2(\kappa R) \approx 1 - \frac{3}{2\kappa R} + \ldots, \tag{66}$$

where the ellipsis imply the terms $\mathcal{O}((\kappa R)^{-2})$.

On another hand, Eq. (57) can be used in (62) in order to obtain an analogue of (63) valid for singular screw dislocations:

$$\sum_{k=1,2} \langle\!\langle \sigma_k^{\rm tot}(\mathbf{x}_1)\, \sigma_k^{\rm tot}(\mathbf{x}_2) \rangle\!\rangle = \frac{\mu}{\beta}(1 + \alpha\mu) \overset{(2)}{\delta}(\mathbf{x}_1 - \mathbf{x}_2)\,. \tag{67}$$

Right-hand sides of (63) and (67) are weakly coinciding at $\kappa^{-1} \to 0$ (i.e., when the core's scale is shrunk). This can be demonstrated by means of integration with an appropriate trial function. Inserting (67) into (62) one obtains:

$$\frac{1}{\mu_{\rm ren}} = \frac{1}{\mu} + \alpha\,. \tag{68}$$

The renormalization rule (68) is in agreement with that obtained in the original paper [4] by means of the macroscopic stress function of collection of the dislocation dipoles. Equation (68) agrees with the renormalization of the shear modulus derived as well in [9, 16] provided low concentration of the defects is considered. As it is seen from (68), increasing of $\alpha$ results in decreasing of $\mu_{\rm ren}$. Clearly, Eq. (64) is reduced to (68) when $\kappa R$ tends to infinity, and so the unit values of the coefficients $\mathcal{C}_1$, $\mathcal{C}_2$ correspond to the case of singular dislocations. Roughly speaking, shrinking up the core regions one goes back to singular dislocations. Notice that the rescaled values of the elastic parameters are used in (64), (68) (i.e., after the replacement $\mu L \to \mu$). Under inverse replacement, $\mu \to \mu L$, Eqs. (64), (68) keep their form except that $\alpha$ (64) is changed to $\alpha L$. Remind that the critical exponents of appropriate correlation functions are analogously renormalized due to presence of the vortex pairs either in the two-dimensional Bose gas [6], or on the string world-sheets [47].

Equation (64) can be re-expressed as follows:

$$\mu \to \mu_{\rm ren} = \frac{\mu}{\mathcal{C}_1(\kappa R)} \Big(1 + \mu\alpha \frac{\mathcal{C}_2(\kappa R)}{\mathcal{C}_1(\kappa R)}\Big)^{-1}\,. \tag{69}$$

At large but finite $\kappa R$ (the scale $1/\kappa$ is small but comparable with the sample's scale $R$), the non-triviality of the dislocation cores finds its implementation in the renormalization of the shear modulus. According to (66), (69), the character of the decreasing of $\mu_{\rm ren}$ is changed in comparison with the case of the singular dislocations: it is slower since $\mathcal{C}_2(\kappa R)/\mathcal{C}_1(\kappa R) < 1$ at large $\kappa R$. It has to be noticed that Eqs. (64) and (69) are valid for non-interacting dipoles (low concentration of the dipoles). Interaction of the dipoles can also be taken into account by means of the formalism developed but should be done elsewhere.

# 5 Discussion

Array of parallel singular screw dislocations is equivalent (as a planar system with respect of the sample's cross-section) to the two-dimensional Coulomb gas of charged point particles. The latter is a subject covered by the theory [1–10, 12–14] of the phase transitions in the low-dimensional systems of condensed matter physics. Dislocations influence re-normalization of the elastic constants of the corresponding material sample. The present paper is to investigate the re-normalization of the shear modulus in the case of the screw dislocations possessing finite-size core regions. The transformation to the Coulomb-like system is used.

The approach [32, 36] admits of finiteness of the dislocation core region, and it is elaborated in the given paper further in order to study collection of the modified screw dislocations as a thermodynamic ensemble. Specifically, a long enough cylindric rod pierced by co-axial non-singular screw dislocations is considered. A field-theoretical formalism is developed to investigate the corresponding partition function in the form of the functional integral. The modified dislocations appear as its stationarity points due to the choice of the energy functional. The plastic external source is involved which governs the background stress distribution. This is a distinct from Refs. [31–34] where the background stress field is pre-imposed by means of, so-called, "null-Lagrangian" postulated.

Calculation of the partition function relates the system of the dislocation dipoles to equivalent description of electrically-neutral Coulomb-like gas of charges interacting *via* potential which is logarithmic at large separation but tends to zero for the charges sufficiently close each to other. The smoothing of the Coulomb potential at short mutual separations between the charges/the dislocations occurs since the self-energy of the cores is accounted for. The stress-stress correlation function of collection of the dislocation dipoles is obtained and used to study the renormalization of the shear modulus. The latter is considered in the approximation of dilute gas of the dislocation dipoles. It is demonstrated that the renormalized shear modulus acquires a non-conventional additional dependence on the characteristic parameter $\kappa R = R/\kappa^{-1}$. Notice that applicability of the effects of renormalization of the elastic constants to experimental observations is discussed in [16].

Since the contributions due to the core demonstrated above are sensible at moderate $\kappa R$, it is hopeful that the formalism developed could be efficient for nanotubes with comparable $R$ and $\kappa^{-1}$. Here importance of the second order stresses within the core region can arise [36]. It is hopeful, [30, 32, 34], that the formalism can be extended to hollow cylinder, as well as developed further for the modified edge dislocations. The latter could be interesting as far as the physics of multi-layer nanotubes and wrapped crystals is concerned [22].

# Acknowledgement

It is a pleasure to express my gratitude to N. M. Bogoliubov, M. Yu. Gutkin, M. O. Katanaev, and A. G. Pronko. The research described has been supported in part by RFBR (Nos. 07-01-00358, 10-01-00600) and by the Russian Academy of Sciences program "Mathematical Methods in Non-Linear Dynamics".

# Appendix

Let us consider the generating functional $\mathcal{G}[\mathbf{J}^{\rm b},\mathbf{J}^{\rm c}\,|\,\boldsymbol{\mathcal{P}}]$ (30) dependent on three 2-component sources, $\mathbf{J}^{\rm b}$, $\mathbf{J}^{\rm c}$, and $\boldsymbol{\mathcal{P}}$:

$$\mathcal{G}[\mathbf{J}^{\rm b},\mathbf{J}^{\rm c}\,|\,\boldsymbol{\mathcal{P}}]\,=\,\int e^{-\beta W+iL\int(J^{\rm b}_i\sigma^{\rm b}_i+J^{\rm c}_j\sigma^{\rm c}_j)\,{\rm d}^2x}\,\mathcal{D}(\sigma^{\rm b}_i,\sigma^{\rm c}_i,u,e_i)\,. \tag{A1}$$

The exponent in (A1) is specified, after fixing the "Coulomb gauge", as follows:

$$\begin{aligned}-\beta W+iL\int(J^{\rm b}_i\sigma^{\rm b}_i+J^{\rm c}_j\sigma^{\rm c}_j)\,{\rm d}^2x\,=\\ =\,\frac{-\beta L}{2\mu}\int\big(\sigma^{\rm b}_i+\sigma^{\rm c}_i\big)^2\,{\rm d}^2x\,-\,2L\beta\ell\int e_i\Delta\,e_i\,{\rm d}^2x\\ +\,iL\int\sigma^{\rm b}_i\big(\partial_i u-2\mathcal{P}_i+J^{\rm b}_i\big)\,{\rm d}^2x\,+\,2L\beta\int\sigma^{\rm c}_i\big(e_i+\frac{i}{2\beta}\,J^{\rm c}_i\big)\,{\rm d}^2x\,.\end{aligned} \tag{A2}$$

It is appropriate to calculate (A1) by shifts of the functional integration variables (this technique is standard, see [14, 37–40]). Interpretation of the stress fields $\sigma^{\rm b}_i$ and $\sigma^{\rm c}_i$ in terms of the background and the gauge contributions is still valuable in the presence of the sources $J^{\rm b}_i$ and $J^{\rm c}_i$. As a first step, the strain field $e_i$ should be integrated out by the shift

$$e_i\,\longrightarrow\,e_i\,-\,\frac{1}{2\ell\Delta}\,\sigma^{\rm c}_i\,.$$

After re-arrangements we obtain for $\mathcal{G}[\mathbf{J}^{\rm b},\mathbf{J}^{\rm c}\,|\,\boldsymbol{\mathcal{P}}]$:

$$\begin{aligned}\mathcal{G}[\mathbf{J}^{\rm b},\mathbf{J}^{\rm c}\,|\,\boldsymbol{\mathcal{P}}]\,\propto\,\int\exp\Bigg[\frac{-\beta L}{2\mu}\int\sigma^{\rm c}_i\,\mathsf{D}^{-1}\sigma^{\rm c}_i\,{\rm d}^2x\,+\,iL\int\sigma^{\rm c}_i\,J^{\rm c}_i\,{\rm d}^2x\\ -\,\frac{\beta L}{2\mu}\int\Big(\sigma^{\rm b}_i\sigma^{\rm b}_i\,-\,i\frac{2\mu}{\beta}\,\sigma^{\rm b}_i\big(\partial_i u-2\mathcal{P}_i+J^{\rm b}_i-\frac{\beta}{i\mu}\sigma^{\rm c}_i\big)\Big)\,{\rm d}^2x\Bigg]\,\mathcal{D}(\sigma^{\rm b}_i,\sigma^{\rm c}_i,u)\,.\end{aligned} \tag{A3}$$

Here '$\propto$' implies that the decoupled integrations, being constant factors which are not of interest now, are included into re-scaling of the integration measure. The kernel $\mathsf{D}^{-1}$ is defined in (A3) as follows:

$$\mathsf{D}^{-1}\,\equiv\,\delta\,-\,\frac{\kappa^2}{\Delta}\,, \tag{A4}$$

where $\Delta^{-1}$ is the Green function of two-dimensional Laplacian, and $\delta$ is the delta-function.

Next step is to shift subsequently the variables $\sigma^{\rm b}_i$ and $\sigma^{\rm c}_i$. To carry out the calculations remaining it is suffice to assume that $J^{\rm b}_i=J^{\rm c}_i=J_i$. Besides, we recall that $\mathcal{P}_i=e^P_i+C_i$. Then, after the shifts

$$\begin{aligned}\sigma^{\rm b}_i\,&\longrightarrow\,\sigma^{\rm b}_i\,+\,\frac{i\mu}{\beta}\,(\partial_i u-2e^P_i+J_i)\,,\\ \sigma^{\rm c}_i\,&\longrightarrow\,\sigma^{\rm c}_i\,-\,\frac{i\mu}{\beta}\,\mathsf{D}(\partial_i u-2e^P_i)\,,\end{aligned} \tag{A5}$$

the generating functional takes the form:

$$\mathcal{G}[\mathbf{J},\mathbf{J}\,|\,\boldsymbol{\mathcal{P}}] \,\propto\, \int \exp\Big[\frac{-\mu L}{2\beta}\int \big((\partial_i u+\mathcal{J}_i)(\delta+\mathsf{D})(\partial_i u+\mathcal{J}_i)+J_i\mathsf{D}J_i$$

$$-2(\partial_i u+\mathcal{J}_i)(\mathsf{D}J_i+2C_i)\big)\,\mathrm{d}^2x \,-\, iL\int \sigma_i^{\mathrm{b}}\big(2C_i-\mathsf{D}(\partial_i u-2e_i^P)\big)\,\mathrm{d}^2x \tag{A6}$$

$$-\,\frac{\beta L}{2\mu}\int(\sigma_i^{\mathrm{c}}\,\mathsf{D}^{-1}\sigma_i^{\mathrm{c}}+\sigma_i^{\mathrm{b}}\sigma_i^{\mathrm{b}}+2\sigma_i^{\mathrm{b}}\sigma_i^{\mathrm{c}})\,\mathrm{d}^2x\Big]\;\mathcal{D}(\sigma_i^{\mathrm{b}},\sigma_i^{\mathrm{c}},u)\,,$$

where the operator $\mathsf{D}$ is inverse to $\mathsf{D}^{-1}$ (A4), and $\mathcal{J}_i\equiv J_i-2e_i^P$.

The experience of the stationary phase estimate in Section 2 demonstrates a necessity of self-consistent choice of the functions $C_i$. The corresponding substitute

$$C_i \,=\, \frac{1}{2}\,\mathsf{D}\,(\partial_i u-2e_i^P) \tag{A7}$$

allows to fix the background contribution and decouples the functional integration over $u$. The latter, in turn, is just responsible for the dependence of the partition function on the plastic strain $e_i^P$ and thus on the defect distribution. The same choice (A7) is suitable for the generating function dependent on the source $\mathbf{J}$. Thus the following representation arises:

$$\mathcal{G}[\mathbf{J},\mathbf{J}\,|\,\boldsymbol{\mathcal{P}}^{\mathrm{ph}}] \,\propto\, \int \exp\Big[\frac{-\mu L}{2\beta}\int\big((\partial_i u+\mathcal{J}_i)(\delta-\mathsf{D})(\partial_i u+\mathcal{J}_i)+J_i\mathsf{D}J_i\big)\,\mathrm{d}^2x\Big]\,\mathcal{D}(u)\,, \tag{A8}$$

where the superscribed notation $\boldsymbol{\mathcal{P}}^{\mathrm{ph}}$ implies that the background distribution of the dislocations is fixed. As a final step, the shift

$$u \,\longrightarrow\, u\,-\,\frac{1}{\Delta}\,\partial_i\mathcal{J}_i\,,$$

allows to get rid of the contribution of the first order in $\partial_i u$. Eventually, the generating functional is given by the following exponential (after $\beta\leftrightarrow 1/\beta$):

$$\mathcal{G}[\mathbf{J},\mathbf{J}\,|\,\boldsymbol{\mathcal{P}}^{\mathrm{ph}}] \,=\, \mathrm{const}\times\,\exp\Big[\frac{-\mu\beta L}{2}\int\Big(\partial_i\mathcal{J}_i\Big(\frac{1}{\Delta}\,-\,\frac{1}{\Delta-\kappa^2}\Big)\partial_k\mathcal{J}_k$$

$$-\,\mathcal{J}_i\,\frac{\kappa^2}{\Delta-\kappa^2}\mathcal{J}_i\,+\,\Delta J_i\frac{1}{\Delta-\kappa^2}J_i\Big)\,d^2x\Big]\,, \tag{A9}$$

where $\mathcal{J}_i\equiv J_i-2e_i^P$. The constant factor denotes all the decoupled integrations. Equation (A9) is just the answer expressed by (32), (33).

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