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Screw dislocations with finite-sized core and the renormalization of the shear modulus near the melting transition*†

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Abstract

Renormalization of the shear modulus caused by dipoles of the screw dislocations lying along infinitely long cylinder is investigated. The core self-energy is taken into account so that the axial singularities of the dislocations are eliminated due to formation of the finite-sized cores. The dipole-dipole coupling is accounted for. The behavior of the renormalized shear modulus is studied, and appropriate implications due to non-singularity of the dislocations are demonstrated near the melting transition.

Key words: dislocation dipole, shear modulus, renormalization, melting
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1 Introduction

The physics of nanotubes/nanowires and of graphene sheets is of importance as far as the development of modern technologies is concerned [1–3]. Dislocations as imperfections of the crystalline ordering have attracted appreciable interest from the viewpoint of real properties of nanostructures [1–10]. For instance, the multilayer nanotubes can contain within their walls screw dislocations lying along the tube axis [8, 9]. The electronic and the mechanical properties of the graphene sheets in presence of dislocations are also of interest [7].

According to the elasticity theory, the stress tensor components of a single dislocation are singular on the defect line since its core is not captured by the classical approach. The dislocation solutions characterized by elimination of the axial singularities have recently been investigated by means of the gradient elasticity and of the gauge-translational approaches (see [11–15] for refs.). This smoothing is due to modification of the conventional solutions within the finite-sized core regions. Since the cross-sectional characteristic scales of the nanotubes are comparable with those of the dislocation cores, effects due to finiteness of the cores look attractive for study from the viewpoint of nanostructures.

Dislocations are of importance also in the theory of melting of two-dimensional systems [16–19] being a part of more general theory of the defect-mediated phase transitions [20–24]. It is crucial that proliferation of the dislocation dipoles is related to the renormalization of the elastic constants [16–19, 21, 25]. Since the nanotubes and the dislocation cores are characterized by comparable radii, it seems attractive to study the renormalization of the elastic constants using the modified dislocation solutions possessing the finite core regions. In this respect, an approach has been developed in [15] in order to evaluate the renormalized shear modulus μ for the screw dislocations with finite-sized core. Free-dipole approximation has been used in [15] to calculate in lowest order with respect to square of the dipole momenta. The present paper is to evaluate the renormalization of μ taking into account the dipole-dipole coupling. The multi-dipole corrections to the renormalization rule are obtained, and influence of the non-conventional character of the dislocation solutions on the renormalization is studied near the melting transition.

The paper is organized as follows. Section 1 is introductive. Section 2 begins with the partition function of the elastic cylinder containing array of the modified screw dislocations. The stress-stress correlation function which incorporates averaging over the dislocation dipole positions is derived in Section 2. Relations characterizing the shear modulus renormalization are studied in Section 3. Discussion in Section 4 closes the paper.

2 The stress-stress correlation function

We consider array of non-singular screw dislocations lying along infinite cylinder as a thermodynamical ensemble at non-zero temperature. The corresponding partition function $\mathcal{Z}$ is written in the functional integral form:

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

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

where β is inverse of the absolute temperature T (the Boltzmann constant is unity), and $\mathcal{D}(\sigma^{\rm b}_{ij}, \sigma^{\rm c}_{ij}, u_i, e_{ij})$ is appropriately normalized integration measure, [15]. Since our framework is that of the plane elasticity, the independence on the third coordinate reduces our study to the two-dimensional problem. Therefore, the functional W (2) consists of the contributions (indices repeated imply summation, $i = 1, 2$):

$$
\begin{aligned}
E_{\rm el} &= \frac{1}{2\mu} \int (\sigma^{\rm b}_i + \sigma^{\rm c}_i)^2 \, {\rm d}^2 x \,, \\
E_{\rm core} &= \int \big(-\ell \,(\partial_i e_j - \partial_j e_i)^2 \; - \; 2 e_i \, \sigma^{\rm c}_i\big) \, {\rm d}^2 x \,, \\
E_{\rm ext} &= \int \sigma^{\rm b}_i (\partial_i u - 2\mathcal{P}_i) \, {\rm d}^2 x \,,
\end{aligned}
\tag{3}
$$

where the integration is over the cylinder's cross-section. Here, $E_{\rm el}$ is the elastic energy of superposition of two stresses, $\sigma^{\rm b}_i$ and $\sigma^{\rm c}_i$, and μ is the shear modulus. The notation $\sigma^{\rm b}_i$ corresponds to the conventional long-ranged dislocation stress, while $\sigma^{\rm c}_i$ is to account for the modification of $\sigma^{\rm b}_i$ within the core. The dislocation core energy is $E_{\rm core}$, the total strain is e_i, and ℓ is the parameter characterizing the core energy. In the two dimensional problem we abbreviate: $\sigma^{\#}_i \equiv \sigma^{\#}_{i3}$ ($\#$ is b or c), $e_i \equiv e_{i3}$, etc. Since the displacement vector of straight screw dislocation is along Ox_3, we use $u \equiv u_3$. The stresses respect the equilibrium equations due to inclusion of the "source" term $E_{\rm ext}$ (3); $E_{\rm ext}$ is also related to the plastic strain e^P_i by means of $\mathcal{P}_i = e^P_i + C_i$. The field e^P_i is to fix a specific configuration of the dislocation lines. Auxiliary field C_i is to ensure self-consistency of the set of equations of the present model.

The partition function $\mathcal{Z}$ (1)–(3) is estimated by steepest descent [15]. For definiteness, consider $\mathcal{N}$ straight screw dislocations intersecting the plane $x_1 O x_2$ at the points $\mathbf{x} = \mathbf{y}_I$ (we use $\mathbf{x} \equiv (x_1, x_2)$), $1 \le I \le \mathcal{N}$, and possessing the Burgers vectors $\mathbf{b}_I$ parallel to Ox_3. Provided the "electro-neutrality" condition $\sum_{I=1}^{\mathcal{N}} b_I = 0$ is imposed, the steepest descent gives the effective energy $\mathcal{W} = \frac{-1}{\beta} \log \mathcal{Z}$ approximately as follows:

$$
\mathcal{W} = \mathcal{W}\big(\{\mathbf{y}_I\}\big) = \frac{-\mu}{4\pi} \sum_{I \neq J} b_I b_J \, \mathcal{U}(\kappa |\mathbf{y}_I - \mathbf{y}_J|) \,, \quad \mathcal{U}(s) \equiv \log\Big(\frac{\gamma}{2} s\Big) \; + \; K_0(s) \,,
\tag{4}
$$

where $\{\mathbf{y}_I\} \equiv \{\mathbf{y}_I\}_{1 \le I \le \mathcal{N}}$ is the set of the dislocation positions, and $\kappa \equiv (\mu/\ell)^{\frac{1}{2}}$. The energy $\mathcal{W}$ (4) demonstrates that the system of the dislocations is equivalent to the electrically-neutral gas of charges interacting through the potential which is logarithmic at large separation but tends to zero for the charges sufficiently close to each other. The smoothing of the Coulomb potential occurs since the self-energy of the cores is accounted for.

Let us turn to the grand-canonical 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. Its partition function in the dipole approximation reads:

$$
\begin{aligned}
\mathbf{Z}_{\rm dip} \;&=\; \sum_{\mathcal{N}=0}^{\infty} \frac{1}{\mathcal{N}!} \prod_{I=1}^{\mathcal{N}} \int {\rm d}^2 \boldsymbol{\xi}_I \int {\rm d}^2 \boldsymbol{\eta}_I \, \exp\Big[-2\beta\mathcal{N}\Lambda - \\
&- \; \beta\Big(\sum_{I=1}^{\mathcal{N}} w(\eta_I) \, + \, \sum_{I<J} w_{IJ}\Big)\Big] \,, \qquad \beta w(\eta) \equiv \mathcal{K}\mathcal{U}(\kappa\eta) \,,
\end{aligned}
\tag{5}
$$

where Λ is the chemical potential per dislocation, and $\mathcal{K} \equiv \frac{\mu\beta}{2\pi}$. Position of $I^{\rm th}$ dipole is given by its center of mass, $\boldsymbol{\xi}_I = (\mathbf{y}_I^+ + \mathbf{y}_I^-)/2$, and momentum, $\boldsymbol{\eta}_I = \mathbf{y}_I^+ - \mathbf{y}_I^-$. Summation over the positions is replaced by the integration. The dipole energy is $w(\eta)$, where $\eta \equiv |\boldsymbol{\eta}|$, while w_{IJ} is the energy of interaction between $I^{\rm th}$ and $J^{\rm th}$ dipoles.

Define two-point stress-stress correlation function $\langle\!\langle \sigma_i^{\rm tot}(\mathbf{x}_1)\, \sigma_j^{\rm tot}(\mathbf{x}_2) \rangle\!\rangle$ (where $\sigma_i^{\rm tot}(\mathbf{x}) = \sigma_i^{\rm b}(\mathbf{x}) + \sigma_i^{\rm c}(\mathbf{x})$) as the following average:

$$\langle\!\langle \sigma_i^{\rm tot}(\mathbf{x}_1)\, \sigma_j^{\rm tot}(\mathbf{x}_2) \rangle\!\rangle \;=\; \mathbf{Z}_{\rm dip}^{-1} \sum_{\substack{\text{numbers of dipoles,}\\ \text{dipole positions}}} \int \sigma_i^{\rm tot}(\mathbf{x}_1)\, \sigma_j^{\rm tot}(\mathbf{x}_2)\, e^{-\beta W_P}\, \mathcal{D}(\sigma_{ij}^{\rm b}, \sigma_{ij}^{\rm c}, u_i, e_{ij})\,. \quad (6)$$

The functional W_P is expressed by (2), (3), and $\mathbf{Z}_{\rm dip}$ is the partition function (5). The index P is to stress that distribution of the dislocation lines is prescribed by means of the plastic strain in the source $\mathcal{P}_i$ ($i = 1, 2$). After evaluation of the functional integral, we obtain from (6):

$$\begin{aligned}\langle\!\langle \sigma_i^{\rm tot}(\mathbf{x}_1)\, \sigma_j^{\rm tot}(\mathbf{x}_2) \rangle\!\rangle \;&=\; \frac{-\mu}{2\pi\beta}\, \partial_{(\mathbf{x}_1)_i} \partial_{(\mathbf{x}_2)_j} \mathcal{U}(\kappa|\mathbf{x}_1 - \mathbf{x}_2|) \\ &+\; \mathbf{Z}_{\rm dip}^{-1} \sum_{\substack{\text{numbers of dipoles,}\\ \text{dipole positions}}} \sigma_i^{\rm tot}(\mathbf{x}_1) \sigma_j^{\rm tot}(\mathbf{x}_2)\, e^{-\beta \mathcal{W}}\,,\end{aligned} \quad (7)$$

where the total elastic stress of a specific distribution of the dislocations, $\sigma_i^{\rm tot}(\mathbf{x})$, is expressed through the corresponding stress potential $\mathcal{U}$:

$$\sigma_i^{\rm tot}(\mathbf{x}) \;=\; \frac{\mu}{2\pi} \sum_I \epsilon_{ki}\, \partial_{(\mathbf{x})_k} \mathcal{U}(\kappa|\mathbf{x} - \mathbf{y}_I^{\pm}|)\,. \quad (8)$$

The dipoles are very compact since the dipole momenta are not too large at small enough temperature: $\langle \boldsymbol{\eta}^2 \rangle \ll \kappa^{-2}$. We use the 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 $L^{\rm th}$ dipole ($1 \le L \le \mathcal{N}$). We follow [26] in order to take into account the dipole-dipole corrections. Therefore the sum in right-hand side of (7) takes the form:

$$\begin{aligned}&\sum_{\text{numbers , positions}} \sigma_i^{\rm tot}(\mathbf{x}_1) \sigma_j^{\rm tot}(\mathbf{x}_2)\, e^{-\beta \mathcal{W}} \;= \\ &= \left(\frac{\mu}{2\pi}\right)^2 \epsilon_{ik}\epsilon_{jl}\, \partial_{(\mathbf{x}_1)_k} \partial_{(\mathbf{x}_2)_l} \sum_{\mathcal{N}=1}^{\infty} \frac{1}{\mathcal{N}!} \prod_{I=1}^{\mathcal{N}} \int \mathrm{d}^2 \boldsymbol{\xi}_I \int \mathrm{d}^2 \boldsymbol{\eta}_I\, e^{-\beta(2\Lambda + w(\eta_I))} \\ &\times \prod_{P<Q} e^{-\beta w_{PQ}} \sum_{K,L=1}^{\mathcal{N}} \mathcal{U}_K^{+-}(\mathbf{x}_1) \mathcal{U}_L^{+-}(\mathbf{x}_2)\,,\end{aligned} \quad (9)$$

where $\mathcal{N}$ is the number of dipoles. The stress potential of $\mathrm{K}^{\rm th}$ dipole observed at the point $\mathbf{x}$, $\mathcal{U}_K^{+-}(\mathbf{x})$, is approximated with regard at $|\boldsymbol{\eta}_K| \ll |\mathbf{x} - \boldsymbol{\xi}_K|$ as follows:

$$\mathcal{U}_K^{+-}(\mathbf{x}) \;\equiv\; \mathcal{U}(\kappa|\mathbf{x} - \mathbf{y}_K^+|) \;-\; \mathcal{U}(\kappa|\mathbf{x} - \mathbf{y}_K^-|) \;\approx\; -\,(\boldsymbol{\eta}_K, \partial_{\mathbf{x}})\, \mathcal{U}(\kappa|\mathbf{x} - \boldsymbol{\xi}_K|)\,, \quad (10)$$

where $(\cdot,\cdot)$ stands for the scalar product of 2-vectors. In order to account for the dipole-dipole couplings, we expand $e^{-\beta w_{PQ}}$ in (9) into the series over w_{PQ}. The dipoles are compact, and therefore non-trivial contributions into (9) are due to the $\tilde{n}$-dipole terms given by the integral [26]:

$$
\begin{aligned}
&\left(\frac{\mu}{2\pi}\right)^2 \epsilon_{ik}\epsilon_{jl}\, \partial_{(\mathbf{x}_1)_k}\partial_{(\mathbf{x}_2)_l} \prod_{I=1}^{\tilde{n}} \int \mathrm{d}^2\boldsymbol{\xi}_I \int \mathrm{d}^2\boldsymbol{\eta}_I\, e^{-\beta(2\Lambda + w(\eta_I))} \\
&\times \mathcal{U}_1^{+-}(\mathbf{x}_1)\,(-\beta w_{12})\,(-\beta w_{23})\ldots(-\beta w_{\tilde{n}-1,\tilde{n}})\,\mathcal{U}_{\tilde{n}}^{+-}(\mathbf{x}_2)\,,
\end{aligned}
\tag{11}
$$

where the dipole-dipole coupling is of the form:

$$
-\beta w_{IJ} \;=\; \mathcal{K}\,(\boldsymbol{\eta}_I, \partial_{\boldsymbol{\xi}_I})(\boldsymbol{\eta}_J, \partial_{\boldsymbol{\xi}_J})\mathcal{U}(\kappa|\boldsymbol{\xi}_I - \boldsymbol{\xi}_J|)\,, \quad \mathcal{K} = \frac{\mu\beta}{2\pi}\,. \tag{12}
$$

In order to proceed with evaluation of (11), we integrate subsequently over $\boldsymbol{\xi}_2$, $\boldsymbol{\eta}_2$, $\boldsymbol{\xi}_3$, $\boldsymbol{\eta}_3$, … (just taking into account (10) and (12), and tacitly assuming that $\tilde{n} \geq 2$). After $k-1$ steps, we obtain:

$$
\begin{aligned}
\mathcal{I}_k \;\equiv\; &\prod_{I=2}^{k} \int \mathrm{d}^2\boldsymbol{\xi}_I \int \mathrm{d}^2\boldsymbol{\eta}_I\, e^{-\beta(2\Lambda + w(\eta_I))} \prod_{J=1}^{k}(-\beta w_{J,J+1}) \;=\; \mathcal{K}^k(-\pi\langle\boldsymbol{\eta}^2\rangle\bar{N})^{k-1} \times \\
&\times (\boldsymbol{\eta}_1, \partial_{\boldsymbol{\xi}_1})(\boldsymbol{\eta}_{k+1}, \partial_{\boldsymbol{\xi}_{k+1}})\Big[\mathcal{U}(\kappa|\boldsymbol{\xi}_1 - \boldsymbol{\xi}_{k+1}|) + \sum_{l=1}^{k-1}(\mathsf{D}_\kappa)^l K_0(\kappa|\boldsymbol{\xi}_1 - \boldsymbol{\xi}_{k+1}|)\Big]\,.
\end{aligned}
\tag{13}
$$

Here D_κ stands for the operator $\frac{-\kappa}{2}\frac{\mathrm{d}}{\mathrm{d}\kappa}$. The $\boldsymbol{\xi}$-integrations in (13) are enabled by the Green theorem [15]. The $\boldsymbol{\eta}$-integrations are expressed in (13) by means of the definition of the mean square of the dipole momentum $\langle\boldsymbol{\eta}^2\rangle$ [21, 26]:

$$
\int e^{-2\beta\Lambda - \mathcal{K}\mathcal{U}(\kappa\eta)}\eta_i\eta_j\,\mathrm{d}^2\boldsymbol{\eta} \;=\; \frac{\delta_{ij}}{2}\langle\boldsymbol{\eta}^2\rangle\bar{N}\,, \tag{14}
$$

where $\bar{N}$ is the average dipole density. The integral (14) diverges at $\mathcal{K} < 4$. The dipolar phase does not exist at the temperature $T > T_c \equiv \frac{\mu}{8\pi}$.

At each intermediate integration over $\boldsymbol{\xi}_I$, $\boldsymbol{\eta}_I$, $1 < I < \tilde{n}$, it is appropriate to keep in right-hand side of (13) only the long-ranged logarithmic contribution thus neglecting the terms decaying fast at $\kappa|\boldsymbol{\xi}_1 - \boldsymbol{\xi}_{I+1}|\gtrsim 1$. Thus we avoid the situation when the distance between positions of compact dipoles is smaller than the characteristic size of the core κ^{-1} [26]. Therefore, Eq. (13) should be written as follows:

$$
\mathcal{I}_k \;\approx\; \mathcal{K}^k(-\pi\langle\boldsymbol{\eta}^2\rangle\bar{N})^{k-1}\,(\boldsymbol{\eta}_1, \partial_{\boldsymbol{\xi}_1})(\boldsymbol{\eta}_{k+1}, \partial_{\boldsymbol{\xi}_{k+1}})\log|\boldsymbol{\xi}_1 - \boldsymbol{\xi}_{k+1}|\,. \tag{15}
$$

After $\tilde{n}-2$ steps, two integrations remain, over $\boldsymbol{\xi}_1$, $\boldsymbol{\eta}_1$, and $\boldsymbol{\xi}_{\tilde{n}}$, $\boldsymbol{\eta}_{\tilde{n}}$. Provided (13) is used, the following expression appears for the whole Eq. (11):

$$
\begin{aligned}
&\left(\frac{\mu}{2\pi}\right)^2 \mathcal{K}^{\tilde{n}-1}(-\pi\langle\boldsymbol{\eta}^2\rangle\bar{N})^{\tilde{n}}\,\epsilon_{ik}\epsilon_{jl}\,\partial_{(\mathbf{x}_1)_k}\partial_{(\mathbf{x}_2)_l}\Big[\mathcal{U}(\kappa|\mathbf{x}_1 - \mathbf{x}_2|) \;+ \\
&\qquad\qquad + \sum_{l=1}^{\tilde{n}}(\mathsf{D}_\kappa)^l K_0(\kappa|\mathbf{x}_1 - \mathbf{x}_2|)\Big]\,.
\end{aligned}
\tag{16}
$$

However, only the term $l = 1$ is to be kept in right-hand side of (16) as far as the relation (15) holds. We take into account $\mathbf{Z}_{\mathrm{dip}}$ (5) and, eventually, obtain (7) in the following form:

$$
\begin{aligned}
\langle\!\langle \sigma_i^{\rm tot}(\mathbf{x}_1)\, \sigma_j^{\rm tot}(\mathbf{x}_2) \rangle\!\rangle \;=\; & \frac{-\mu}{2\pi\beta}\, \partial_{(\mathbf{x}_1)_i}\partial_{(\mathbf{x}_2)_j}\mathcal{U}(\kappa|\Delta\mathbf{x}|) \\
+\, \frac{\mu}{2\pi\beta} \sum_{\tilde{n}=1}^{\infty} (-\beta\mu d)^{\tilde{n}} & \left(\epsilon_{ik}\epsilon_{jl}\, \partial_{(\mathbf{x}_1)_k}\partial_{(\mathbf{x}_2)_l}\right) \Big[\mathcal{U}(\kappa|\Delta\mathbf{x}|) + \frac{\kappa|\Delta\mathbf{x}|}{2}\, K_1(\kappa|\Delta\mathbf{x}|)\Big]\,,
\end{aligned}
\tag{17}
$$

where $\Delta\mathbf{x} \equiv \mathbf{x}_1 - \mathbf{x}_2$, and the contribution at $\tilde{n} = 1$ just corresponds to [15]. Besides, we introduced d by means of the relation: $\beta\mu d \equiv \pi\mathcal{K}\langle\boldsymbol{\eta}^2\rangle\bar{N}$. The parameter d is proportional to mean area covered by the dipoles.

3 The renormalization of the shear modulus

Let us obtain the renormalized shear modulus $\mu_{\rm ren}$, which is expressed through the average (6) as follows [18, 25]:

$$
\frac{1}{\mu_{\rm ren}} \;\equiv\; \frac{\beta}{\mu^2\mathcal{S}} \sum_{i,k} \iint \langle\!\langle \sigma_i^{\rm tot}(\mathbf{x}_1)\, \sigma_k^{\rm tot}(\mathbf{x}_2) \rangle\!\rangle \, \mathrm{d}^2\mathbf{x}_1 \mathrm{d}^2\mathbf{x}_2\,, \tag{18}
$$

where $\mathcal{S}$ is the area of the sample's cross-section. The main relation of the present paper arises from (17) and (18):

$$
\frac{1}{\mu_{\rm ren}} \;=\; \frac{1}{\mu}\,\mathcal{C}_1(\kappa R) \;+\; \frac{\beta d}{1+\beta\mu d}\,\mathcal{C}_2(\kappa R)\,, \tag{19}
$$

where $\mathcal{C}_1(z) = 1 - 2K_1(z)I_1(z)$ and $\mathcal{C}_2(z) = \mathcal{C}_1(z) + \mathsf{D}_z\mathcal{C}_1(z)$ are given by the modified Bessel functions. When μd is not too large, $\mu d \ll 1$, the renormalization rule (19) is reduced to the relation obtained in [15]. Equation (19) demonstrates that the shear modulus $\mu_{\rm ren}$ depends on the ratio R/κ^{-1} of the sample's cross-section radius to that of the dislocation core. The coefficients $\mathcal{C}_1(z)$ and $\mathcal{C}_2(z)$ both are positive and less than unity. They behave at growing z as follows: $\mathcal{C}_1(z) \approx 1 - \frac{1}{z} + \frac{3}{8z^3} - \ldots$ and $\mathcal{C}_2(z) \approx 1 - \frac{3}{2z} + \frac{15}{16z^3} - \ldots$. Equation (19) corresponds to the case of singular dislocations when κR tends to infinity (see, for comparison, Eq. (59) in [25] obtained however for three-dimensional solid).

According to the rule (19), the ratio $\frac{\mu_{\rm ren}}{\mu}$ is characterized by the following double-sided estimate:

$$
\frac{1}{2} \le \frac{1}{\mathcal{C}_1 + \mathcal{C}_2} < \frac{\mu_{\rm ren}}{\mu} = \frac{1+\beta\mu d}{\mathcal{C}_1 + \beta\mu d\,(\mathcal{C}_1+\mathcal{C}_2)} < \frac{1}{\mathcal{C}_1}\,. \tag{20}
$$

Let $\tilde{\mu}_{\rm ren}$ to denote the renormalized shear modulus in the case of singular dislocations (when $\mathcal{C}_{1,2} = 1$). Then, one obtains from (20) that $\tilde{\mu}_{\rm ren} < \mu_{\rm ren}$ and $\frac{1}{2} < \tilde{\mu}_{\rm ren}/\mu < 1$. Since $\mathcal{C}_{1,2}$ are positive and less than unity, certain restrictions must be fulfilled in order to make (20) physically meaningful. First of all, in order to avoid the contradiction with $\mu_{\rm ren}/\mu < 1$, we require $\mathcal{C}_1 + \mathcal{C}_2 > 1$. The latter is valid at $\kappa R \gtrsim 2.17$. Therefore, the series expansions of $\mathcal{C}_{1,2}(z)$ are admissible provided the value of $\frac{1}{z}$ respects the estimate: $0 < \frac{1}{z} \le \frac{1}{2.17} \approx 0.46$. External diameter of the nanotubes ranges from nanometers to tens of nanometers. As an example, let us specify the cylinder's radius R as follows: $R \lesssim 10\,a$, where a is lattice spacing. We know that $\frac{1}{\kappa} \simeq 0.25a$, according to [11], and thus $\kappa R \lesssim 40$, or $\frac{1}{\kappa} \simeq 0.4a$, according to [14], and so $\kappa R \lesssim 25$. Thus, an admissible range is determined for κR.

Furthermore, the leading contribution to $\mu_{\rm ren}/\mu$ is $(\mathcal{C}_1+\mathcal{C}_2)^{-1}$ provided the dislocation density μd is large enough. For instance, $(\mathcal{C}_1+\mathcal{C}_2)^{-1}$ is 0.72 at $\kappa R = 4.0$, or 0.55 at $\kappa R = 15.0$, or 0.53 at $\kappa R = 25.0$. Besides, $\mu_{\rm ren}/\mu$ reduces to $\frac{1}{\mathcal{C}_1}$ provided μd decreases. Since $\frac{1}{\mathcal{C}_1} > 1$, it is appropriate to ensure $\mu_{\rm ren}/\mu < 1$ requiring the validity of the inequalities:

$$\frac{1+\beta\mu d}{\mathcal{C}_1(z)+\beta\mu d(\mathcal{C}_1(z)+\mathcal{C}_2(z))} < 1 \iff f(z) \equiv \frac{1-\mathcal{C}_1(z)}{\mathcal{C}_1(z)+\mathcal{C}_2(z)-1} < \beta\mu d\,. \tag{21}$$

Therefore, the inequality $f(z) < \beta\mu d$, Eq. (21), imposes the lower bound in the sense that $\beta\mu d$ should not lie below $f(z)$ (see *Fig. 1*) provided z acquires admissible values. One can also compare the dependence of $\mu_{\rm ren}/\mu$ on $\beta\mu d$ in the singular and non-singular cases (see *Fig. 2* drawn for $\kappa R = 15.0$).

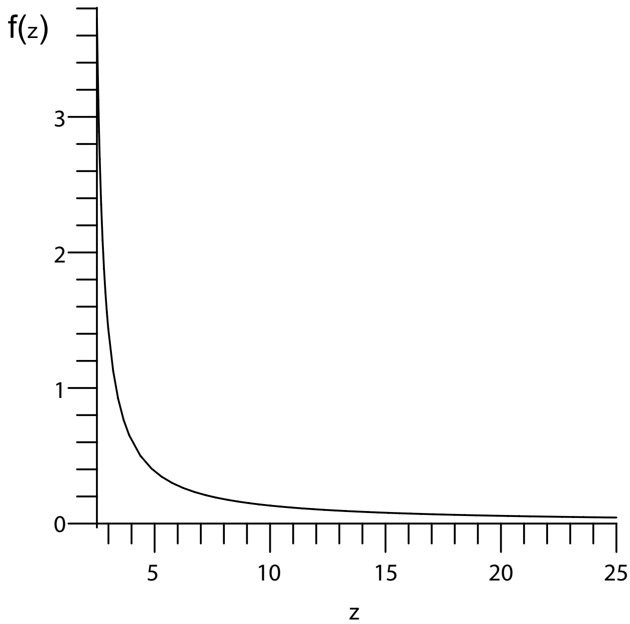

Figure 1: $f(z)$

The rule (19) enables one to express the renormalized shear modulus as the function of the absolute temperature, $\mu_{\rm ren} = \mu_{\rm ren}(T)$. The temperature T_c of the melting transition is given by (14), and it respects $\mu\beta_c = 8\pi$. The function $\mu_{\rm ren}(T)$ takes the following form in a close vicinity of T_c (at $T < T_c$):

$$\frac{\mu_{\rm ren}(T)}{\mu_{\rm ren}(T_c^-)} \approx 1 + \Big(\frac{T}{T_c} - 1\Big) h(\kappa R)\,, \qquad h(\kappa R) \equiv \frac{8\pi d}{(1+8\pi d)(8\pi d + \mathcal{C}^*(\kappa R)(1+8\pi d))}\,, \tag{22}$$

where $\mathcal{C}^*(\kappa R) \equiv \frac{\mathcal{C}_1(\kappa R)}{\mathcal{C}_2(\kappa R)}$. The limits $\mathcal{C}^*(\kappa R) \to 1$ and $h(\kappa R) \to h_\infty$ take place at $\kappa R \to \infty$, and this corresponds to the case of singular dislocations. Numerical estimate shows us that $1.0 < \mathcal{C}^*(\kappa R) < 1.4$ at $\kappa R > 2.17$, and so $h(\kappa R)$ is smaller than the limiting value h_∞. The limiting value of $\mu_{\rm ren}(T)$ below the critical temperature, $\mu_{\rm ren}(T_c^-)$, is also

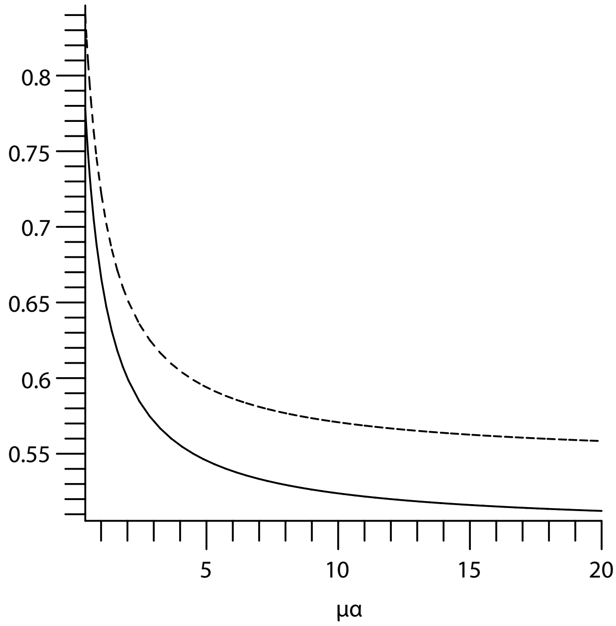

Figure 2: $\mu_{\rm ren}/\mu$ (dashed) and $\tilde{\mu}_{\rm ren}/\mu$ *vs* $\mu\alpha \equiv \beta\mu d$

obtainable from (19) ($\mu_{\rm ren}$ is zero above the transition point). The value of $\mu_{\rm ren}(T_c^-)$ can be compared with the analogous value for the singular dislocations. It is appropriate to put the corresponding inequality in the following form:

$$\frac{\mu_{\rm ren}(T_c^-)}{T_c} = \frac{8\pi(1+8\pi d)}{\mathcal{C}_1 + 8\pi d(\mathcal{C}_1 + \mathcal{C}_2)} > \frac{\tilde{\mu}_{\rm ren}(T_c^-)}{T_c} = \frac{8\pi(1+8\pi d)}{1+16\pi d}\,. \tag{23}$$

Crucially, Eq. (23) demonstrates that the value of $\frac{\mu_{\rm ren}(T_c^-)}{T_c}$ at $d \ll 1$ (or $d \gg 1$) ceases to be an integer multiplied by π, as it happens for $\frac{\tilde{\mu}_{\rm ren}(T_c^-)}{T_c}$.

Therefore, Eqs. (22) and (23) demonstrate how the non-conventional character of the dislocation solution influences, through the dependence on $\mathcal{C}_1(\kappa R)$, $\mathcal{C}_2(\kappa R)$, the shear modulus renormalization near the melting transition. It should be noticed that a direct verification of the limiting value of the Young modulus (which is 16π at $T \to T_c^-$) predicted by the theory [16–19] has been reported in [27], where the two-dimensional colloidal crystal has been used. More references concerning testing of the essential elements of the theory [16–19] can also be found in [27]. Appropriate candidates for observing the effects of the elastic constants renormalization have been discussed in [25], where the colloidal crystals have also been mentioned as the suitable ones.

4 Discussion

The renormalization of the shear modulus is studied in the case of the screw dislocations possessing the finite-sized core. The influence of the dipole-dipole interaction on the renormalization rule is taken into account. Approximation of compact dipoles is used.

The non-triviality of the cores is valuable for the renormalization of the shear modulus at finite κR. The numerical restrictions ensuring the validity of (19) are not in contradiction with realistic characteristics of the nanotubes/nanowires. The relations obtained, (19), (22), (23), demonstrate the thermodynamical implications of the usage of the singularityless modified dislocation solutions. Although the effects of the renormalization a very subtle, the nanophysics could hopefully provide an opportunity to verify the corresponding predictions of the approach proposed to elimination of the dislocation singularities. Further development for nonsingular edge dislocations should be interesting.

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