Statistical physics of interacting dislocation loops and their effect on the elastic moduli of isotropic solids

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We present a field-theoretical study of interacting dislocation loops and their effect on the elastic moduli of isotropic three-dimensional solids. We find that the shear modulus decreases to a finite limit with increasing density and size of dislocation loops and vanishes only with the appearance of open dislocation lines that terminate on the boundaries of the sample. Using the random phase approximation, we analyze the correlations of dislocation ''charges'' and ''currents'' and show that interaction between dislocations leads to screening of long-range correlations. Variational and perturbative methods are used to show that fluctuation-induced attraction between segments of dislocation loops leads to the shrinking of the radii of gyration of loops compared to their Gaussian dimensions. The applicability of our model assumptions to real solids is discussed. [S0163-1829(99)03121-5]

I. INTRODUCTION

Following the pioneering work of Kosterlitz and Thouless[1] on vortex unbinding in the xy model, the statistical physics of topological defects in solids attracted considerable attention in the theoretical physics community. Although the original work as well as its extension to dislocation-induced melting of solids by Nelson and Halperin[2] was restricted to $2d$, there was hope that similar ideas can be applied to the melting of $3d$ crystals.[3] Using a simplified form for the interaction between dislocations to construct a free energy as a function of the dislocation density, Edwards and Warner[4] showed that the screening of the interaction leads to a first-order solid-to-liquid transition. Nelson and Toner[5] assumed that such melting does take place and showed that it leads to a liquid state that has some degree of orientational order. A first-order melting transition was also predicted using field-theoretical methods that utilized the analogy with electrodynamics (the interaction between dislocations is mediated by the stress field, just like the interaction between currents is mediated by the magnetic field) by Kleinert[6] and by Obukhov.[7] All of the above-mentioned works were primarily concerned with the analysis of the dislocation-induced melting transition and of its consequences and a thermal distribution of dislocations was always assumed. Note, however, that since in most solids the core energies of dislocations far exceed the available thermal energy, such defects can not be produced by thermal fluctuations.[8]

Here, we take a different path. Throughout most of this paper it is assumed that some given distribution of dislocations (in terms of their lengths and Burgers vectors) is fixed by some nonequilibrium method of preparation, and that thermal equilibrium is attained only with respect to the conformations of the dislocations and their positions in the solid. We then proceed to analyze the effect of this distribution of dislocations on the elastic moduli of the solid and, in the process, obtain interesting insights into the physics of interacting dislocation loops.

In Sec. II, we present a brief review of the continuum theory of dislocations in isotropic solids. In Sec. III, we show that the renormalization of the tensor of elastic constants due to the presence of dislocations can be reduced to the calculation of the correlation function of dislocation ''charges.'' The charge-charge correlation function of noninteracting dislocations is calculated in Appendix A. In Sec. IV, we introduce a field-theoretical formulation of the problem of interacting dislocation loops and use it to study the effect of long-range interactions on the correlations of dislocation ''currents'' and ''charges'' and to calculate the renormalized elastic moduli within the random phase approximation (details of the calculation are given in Appendix B). In Sec. V we derive the free energy and calculate the equilibrium distribution of dislocations. In Sec. VI, we use a variational approach to study the fluctuation-induced attraction between segments of dislocation loops and estimate the resulting compression of the loops and its effect on the thermodynamics and the elastic moduli. In Appendix C, we present a perturbative calculation of the interaction-induced corrections to the radii of gyration of large dislocation loops and show that the results are in good agreement with the variational estimate of Sec. VI. Finally, in Sec. VII we discuss the main results of this paper and comment on its experimental ramifications.

II. CONTINUUM THEORY OF DISLOCATIONS

We begin with a review of the main results of the continuum theory of dislocations in homogeneous and isotropic solids.[9] Within the framework of the linear theory of elasticity, the free energy is given by

$$F_{el}[\mathbf{u}]=\frac{\mu}{2}\int d^3x\left(u_{ik}^2+\frac{\nu}{1-2\nu}u_{ll}^2\right), \tag{1}$$

where μ is the shear modulus, ν is the Poisson ratio, and the strain tensor u_{ik} is defined in terms of the displacement field $\mathbf{u}(\mathbf{x})$

$$u_{ik}=\frac{1}{2}\left(\frac{\partial u_i}{\partial x_k}+\frac{\partial u_k}{\partial x_i}\right). \tag{2}$$

Here and later the usual summation convention regarding repeated indices is used.

We now consider the equilibrium state of the solid, with no externally applied stress on its surface. In the absence of dislocations the stress and the displacement fields vanish everywhere inside the solid. The introduction of dislocations results in singularities in the stress field and the displacement field $\mathbf{u}^{dis}(\mathbf{x})$ becomes a multivalued function of $\mathbf{x}$. The contour integral of $\mathbf{u}^{dis}(\mathbf{x})$ taken around the dislocation line is the Burgers vector $\mathbf{b}$ of the dislocation[9]

$$\oint d\mathbf{u}^{dis}=-\mathbf{b} \tag{3}$$

$\mathbf{u}^{dis}(\mathbf{x})$ is found from the equations of equilibrium of the solid

$$\partial\sigma_{ik}^{dis}/\partial x_k=0, \tag{4}$$

where

$$\sigma_{ik}^{dis}=2\mu\left(u_{ik}^{dis}+\frac{\nu}{1-2\nu}\delta_{ik}u_{ll}^{dis}\right) \tag{5}$$

is the stress tensor. Instead of considering $\mathbf{u}^{dis}(\mathbf{x})$ as a multivalued function, it is more convenient to regard it as a single-valued function of the position, which has discontinuities on surfaces associated with dislocation loops in the bulk of the solid. Due to the linearity of these equations the displacement field $\mathbf{u}^{dis}(\mathbf{x})$ can be represented as the sum of contributions of different dislocation loops C

$$\mathbf{u}^{dis}(\mathbf{x})=\sum_C \mathbf{u}^C(\mathbf{x}). \tag{6}$$

The solution for the displacement vector in the presence of a dislocation loop C with Burgers vector $\mathbf{b}^C$ can be conveniently written down using the Fourier transform

$$\mathbf{u}(\mathbf{x})=\int\frac{d^3q}{(2\pi)^3}\tilde{\mathbf{u}}(\mathbf{q})e^{i\mathbf{q}\cdot\mathbf{x}}. \tag{7}$$

We get (the derivation of the corresponding coordinate space expressions is given in Ref. 9)

$$\tilde{\mathbf{u}}^C(\mathbf{q})=-\mathbf{b}^C\tilde{\omega}^C(\mathbf{q})+\frac{1}{q^2}\left(\mathbf{1}-\frac{1}{1-\nu}\frac{\mathbf{qq}}{q^2}\right)\cdot\tilde{\mathbf{f}}^C(\mathbf{q}), \tag{8}$$

where

$$\tilde{\mathbf{f}}^C(\mathbf{q})\equiv\mathbf{b}^C\times\tilde{\mathbf{j}}^C(\mathbf{q}),\quad \tilde{\mathbf{j}}^C(\mathbf{q})=\oint_C d\mathbf{x}e^{-i\mathbf{q}\cdot\mathbf{x}} \tag{9}$$

and the integration goes over the contour of the dislocation line. The Fourier transform of $\tilde{\mathbf{f}}^C(\mathbf{q})$ can be interpreted as an effective force exerted on the elastic medium by the dislocation C.

The nonuniqueness of the function $\tilde{\mathbf{u}}^C$ is contained entirely in the term $\tilde{\omega}^C$. The Fourier transform of the gradient of ω^C is determined by the configuration of the dislocation line

$$\int d^3xe^{-i\mathbf{q}\cdot\mathbf{x}}\nabla\omega^C=\frac{i}{q^2}\mathbf{q}\times\tilde{\mathbf{j}}^C(\mathbf{q}). \tag{10}$$

Note that for finite-size loops the function ω^C is $1/4\pi$ of the solid angle $\Omega^C(\mathbf{x})$ through which the loop is seen from the point $\mathbf{x}$,

$$\Omega^C(\mathbf{x})\equiv-\int_{S_C}\frac{(\mathbf{x}-\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|^3}\cdot d\mathbf{f}'. \tag{11}$$

Here the integration goes over some arbitrarily chosen discontinuity surface S_C spanning the dislocation loop C. The discontinuity of $\mathbf{u}^C(\mathbf{x})$ across this surface is just the Burgers vector $\mathbf{b}^C$ of the dislocation C.

The function $\tilde{\mathbf{j}}^C(\mathbf{q})$ defined in Eq. (9) is the Fourier component of the conserved dislocation current of loop C

$$\mathbf{j}^C(\mathbf{x})\equiv\oint_C ds\frac{d\mathbf{x}(s)}{ds}\delta[\mathbf{x}-\mathbf{x}(s)],\quad \nabla\cdot\mathbf{j}^C(\mathbf{x})=0, \tag{12}$$

where a parametrization $\mathbf{x}(s)$ along the dislocation line is chosen. The constraint of current conservation (in its Fourier-transformed form), $\mathbf{q}\cdot\tilde{\mathbf{j}}^C=\mathbf{0}$, follows directly from the definition Eq. (9) and expresses the fact that a dislocation must be either a closed loop or an infinite line that terminates at the boundaries of the solid. Since dislocation currents are going to play a major role in our considerations, it is important to get some intuition about their physical meaning. From its definition, Eq. (12), the dislocation current associated with a given dislocation loop C at a point x does not vanish only on the contour of the loop. When x coincides with a point s of the contour, the current at this point is the unit tangent vector to the dislocation $\tau(s)=dx(s)/ds$. Since any smooth curve is completely defined by the collection of tangent vectors at each point of its contour, specification of the current gives complete information about the conformation of the dislocation loop.

III. RENORMALIZATION OF ELASTIC MODULI

In the following we consider a solid with a given distribution $\{n(\mathbf{b},N)\}$ of dislocations, where $n(\mathbf{b},N)$ is the number of dislocations with Burgers vector $\mathbf{b}$ and contour length N. In order to calculate the elastic constants of the solid in the presence of dislocations we follow the approach of Ref. 2, which is based on the linear-response relation between the reaction of a solid to stresses applied to its boundaries and its thermal fluctuations. The first type of fluctuations corresponds to displacement and change of shape of the contours of the dislocations and satisfies the equilibrium condition Eq. (4). This contribution, $\mathbf{u}^{dis}(\mathbf{x})$, is defined by Eqs. (6) and (8) and has discontinuities on the surfaces associated with the dislocation loops. We also consider the thermal fluctuations of the solid (phonons) for a given configuration of the dislocations, that can be described by a smoothly varying displacement field $\phi(\mathbf{x})$. The total displacement field due to fluctuations is the sum of the above contributions,

$$\mathbf{u}(\mathbf{x})=\mathbf{u}^{dis}(\mathbf{x})+\phi(\mathbf{x}). \tag{13}$$

Substituting Eqs. (13) and (4) into Eq. (1), we find that the two types of fluctuations are orthogonal to each other in the sense that the free energy can be decomposed into two independent parts

$$F=F_{el}[\phi]+F_{el}[\mathbf{u}^{dis}]. \tag{14}$$

The free energy associated with the smoothly varying displacement field can written in the form

$$F_{el}[\phi]=\frac{1}{2}\int d^3x\,\phi_{ij}\lambda_{ij\,kl}\phi_{kl}, \tag{15}$$

where ϕ_{ij} is defined by Eqs. (13) and (2) and the tensor of ''bare'' elastic constants (i.e., those of a dislocation-free solid) is

$$\lambda_{ij\,kl}=\mu\left(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk}+\frac{2\nu}{1-2\nu}\delta_{ij}\delta_{kl}\right), \tag{16}$$

with δ_{ij} the Kronecker tensor.

We proceed to examine the renormalization of the elastic constants μ and ν by the presence of dislocations. The inverse tensor of the renormalized elastic constants can be expressed in terms of the correlation function,[2]

$$(\lambda_R^{-1})_{ij\,kl}=\frac{1}{VT}\langle U_{ij}U_{kl}\rangle. \tag{17}$$

Here, V is the volume of the solid, T is the temperature, and

$$U_{ij}=\frac{1}{2}\left(\int df_i u_j+\int df_j u_i\right), \tag{18}$$

where the integration goes over the surface of the sample. Note that U_{ij} has the dimensions of volume and its trace is the volume change of the body due to thermodynamic fluctuations. Equation (17) is derived by considering the response of $\langle U_{ij}\rangle$ to infinitesimal external stress, treating each component of U_{ij} as an independent fluctuating variable.

Inserting the decomposition Eq. (13) into Eq. (18) and using the orthogonality of the smoothly varying and singular parts Eq. (14) we get

$$(\lambda_R^{-1})_{ij\,kl}=(\lambda^{-1})_{ij\,kl}+\frac{1}{VT}\langle U_{ij}^{dis}U_{kl}^{dis}\rangle, \tag{19}$$

where U_{ij}^{dis} is the dislocation contribution to U_{ij} and the tensor

$$(\lambda^{-1})_{ij\,kl}=\frac{1}{VT}\left\langle\int d^3x\,\phi_{ij}(\mathbf{x})\int d^3x'\,\phi_{kl}(\mathbf{x}')\right\rangle$$
$$=\frac{1}{4\mu}\left(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk}-\frac{2\nu}{1+\nu}\delta_{ij}\delta_{kl}\right) \tag{20}$$

is the inverse of the tensor of the bare elastic constants (16), i.e., $(\lambda^{-1})_{ij\,kl}\lambda_{kl\,mn}=\frac{1}{2}(\delta_{im}\delta_{jn}+\delta_{in}\delta_{jm})$.

The application of Gauss' theorem to Eq. (18) yields

$$U_{ij}^{dis}=\int d^3x\,u_{ij}^{dis}(\mathbf{x}),\quad u_{ij}^{dis}(\mathbf{x})=\tfrac{1}{2}(w_{ij}+w_{ji}),$$
$$w_{ij}\equiv\frac{\partial u_j^{dis}}{\partial x_i}. \tag{21}$$

Strictly speaking, this is valid only if there are no surface singularities, i.e., no dislocations that terminate on the surface of the sample. However, the contribution from finite loops that lie near the boundary is much smaller than that of those inside the volume and becomes negligible in the thermodynamic limit. The argument breaks down in the presence of a nonvanishing concentration of infinite dislocation lines that terminate on the surface of the solid. As will be shown in the following, in this case the solid is no longer able to sustain shear and liquidlike behavior results.

In principle, one can proceed as in Ref. 2 and decompose U_{ij}^{dis} into a contribution of the smoothly varying part of $u_{ij}^{dis}(\mathbf{x})$ [terms proportional to $\tilde{\mathbf{f}}^C$ in Eq. (8)], and a contribution $d_{ij}+d_{ji}$ of the discontinuities [the term proportional to $\tilde{\omega}^C$ in Eq. (8)] across the surfaces $\{S_C\}$

$$d_{ij}\equiv\sum_C b_i S_j(C),\quad S_j(C)\equiv\int_{S_C}df_j=\frac{1}{2}\varepsilon_{jkl}\oint_C x_k dx_l, \tag{22}$$

where ε_{ijk} is the antisymmetric unit tensor and d_{ij} is the dislocation moment tensor. The axial vector $S(C)$ has components equal to the areas bounded by the projections of the loop C on planes perpendicular to the corresponding coordinate axes.

Instead of using this decomposition, we relate w_{ij} to the configurations of the dislocation loops [i.e., to the dislocation currents j^C defined in Eq. (12)]. We Fourier transform Eq. (8) to real space, apply the gradient to both sides of the equation and Fourier transform back to q space. Using the relations Eqs. (6) and (10) yields

$$\tilde{w}_{ij}(\mathbf{q})=S_{ij\,i'j'}(\mathbf{q})\tilde{\alpha}_{i'j'}(\mathbf{q}),$$
$$S_{ij\,i'j'}(\mathbf{q})=\frac{i}{q}\left(\delta_{ij'}C_{ji'}-\frac{q_i}{q}\varepsilon_{ji'j'}+\frac{1}{1-\nu}\frac{q_iq_j}{q^2}C_{i'j'}\right), \tag{23}$$

where

$$C_{jk}\equiv\varepsilon_{jkm}q_m/q \tag{24}$$

and $\tilde{\alpha}_{i'j'}(\mathbf{q})$ is the Fourier transform of the dislocation ''charge'' tensor (we adopt the terminology of Ref. 5 since the Burgers vector can be considered as a topological charge), defined as the sum over the contributions of different loops, each of which is the product of the dislocation current by the corresponding Burgers vector

$$\alpha_{ij}(\mathbf{x})=\sum_C j_i^C(\mathbf{x})b_j^C. \tag{25}$$

Thus, the dislocation charge tensor contains complete information about the configurations of the loops, weighted by the appropriate Burgers vectors. Taking the trace of the tensor $\tilde{w}_{ij}$, Eq. (23), we obtain

$$\tilde{w}_{ii}(\mathbf{q}) = -\frac{i}{q}\frac{1-2\nu}{1-\nu}C_{i'j'}\tilde{\alpha}_{i'j'}(\mathbf{q}). \quad (26)$$

Note that w_{ii} describes the volume change due to the presence of dislocations, which vanishes when $\nu=\frac{1}{2}$ (incompressible solid).

Substituting Eq. (23) into Eq. (21), we finally get

$$\frac{1}{V}\langle U_{ij}^{dis}U_{kl}^{dis}\rangle = \lim_{q\to 0}\,\Xi_{(ij)\,(kl)}(\mathbf{q}),$$

$$\Xi_{ij\,kl}(\mathbf{q}) \equiv S_{ij\,i'j'}(\mathbf{q})S_{kl\,k'l'}(-\mathbf{q})\tilde{D}_{i'j'k'l'}(\mathbf{q}), \quad (27)$$

where brackets (ij) and (kl) denote symmetrization over indices ij and kl respectively and $\tilde{D}_{i'j'k'l'}(\mathbf{q})$ is the Fourier transform of the charge-charge correlation function

$$D_{ij\,kl}(\mathbf{x}-\mathbf{x}') \equiv \langle \alpha_{ij}(\mathbf{x})\alpha_{kl}(\mathbf{x}')\rangle \quad (28)$$

In the next section we calculate this correlation function using the field-theoretical formulation of the problem of interacting dislocation loops.

IV. GAUGE FIELD THEORY OF DISLOCATIONS

We proceed to evaluate the partition function of a solid that contains a given distribution of dislocation loops. The presence of dislocation loops results in the distortion of the solid in which they are embedded. It is convenient to replace the above ''geometrical'' picture of a deformed medium by that of interacting dislocation charges and to introduce a local field that mediates the (intra and interloop) interactions between the segments of the dislocation loops, in close analogy to the role played by the electromagnetic field, which mediates the interaction between charges in electrodynamics.[6,7] This is achieved by the following Hubbard-Stratonovitch transformation[10]

$$\exp(-F_{el}[\mathbf{u}^{dis}]/T) = \int D\sigma\,\exp(\hat{F}[\sigma]/T) \times \exp\left[\frac{1}{T}\sum_C \int d\mathbf{x}\,\sigma_{ik}(\mathbf{x})u_{ik}^C(\mathbf{x})\right]. \quad (29)$$

Here $F_{el}[\mathbf{u}^{dis}]$ is the elastic free energy, T is the temperature and the integration goes over the stress-tensor-like field σ_{ik} which is taken to be symmetric and divergenceless (this reduces the number of independent components of σ to three, the number of components of the displacement vector $\mathbf{u}^{dis}$). $\hat{F}[\sigma]$ is the deformation energy for a given σ_{ik}:

$$\hat{F}[\sigma] = \int d^3x\frac{1}{4\mu}\left(\sigma_{ik}^2 - \frac{\nu}{1+\nu}\sigma_{ll}^2\right). \quad (30)$$

Note that in order for the integral, Eq. (29), to be well defined we have to integrate over a purely imaginary tensor field σ_{ik}. The steepest descent evaluation of this functional integral (which is exact for Gaussian integrals) is done by deforming the integration contour from the imaginary σ_{ik} axis, around the segment $[0,\sigma_{ik}^{dis}(\mathbf{u}^{dis})]$ of the real σ_{ik} axis. The steepest descent value, $\sigma_{ik}^{dis}(\mathbf{u}^{dis})$, can be identified with the physical stress tensor, Eq. (5).

A convenient parametrization of this field was proposed in Ref. 6

$$\sigma_{ik} = i\varepsilon_{ijl}\varepsilon_{kmn}\nabla_j\nabla_m h_{ln} = iT\varepsilon_{ijl}\nabla_j A_{lk}$$

$$A_{lk} \equiv \frac{1}{T}\varepsilon_{kmn}\nabla_m h_{ln}, \quad (31)$$

where $h_{ln}(\mathbf{x})$ is a real symmetric tensor field. By construction, σ_{ik}, A_{lk}, and $\hat{F}$ are invariant under the local gauge transformations

$$h_{ik} \to h_{ik} - \nabla_i\Lambda_k - \nabla_k\Lambda_i,$$

$$A_{lk} \to A_{lk} - \nabla_l\varphi_k, \quad \varphi_k = \frac{1}{T}\varepsilon_{kmn}\nabla_m\Lambda_n, \quad (32)$$

where $\mathbf{\Lambda}(\mathbf{x})$ is an arbitrary vector field. To integrate over the fields h_{ik} we must fix a gauge condition, which we choose in the form $\nabla_i h_{ik}=0$. According to Eq. (31), this condition corresponds to the ''Coulomb'' gauge $\nabla_i A_{ik}=0$ and the free energy (30) takes an especially simple form

$$F_0[\mathbf{h}] \equiv -\hat{F}[\sigma] = \int d^3x\frac{1}{4\mu}\left\{(\Delta h_{ik})^2 - \frac{\nu}{1+\nu}(\Delta h_{ll})^2\right\}. \quad (33)$$

The term linear in u_{ik}^C in Eq. (29) can rewritten in the form

$$\int d^3x\,\sigma_{ik}u_{ik}^C = \int d^3x\,\sigma_{ik}\nabla_i u_k^C = \int d^3x\,\nabla_i(u_k^C\sigma_{ik}) = iTb_k^C\oint_C dx_l A_{lk}, \quad (34)$$

where we have used the condition $\nabla_i\sigma_{ik}=0$ to derive the second equality in Eq. (34). The last equality in this equation was derived using Gauss' theorem and noticing that since the normal component of σ_{ik} vanishes on the boundary of the solid, the only contribution to the integral comes from the discontinuity $b_k^C\sigma_{ik}$ of the function $u_k^C\sigma_{ik}$ at the surface S_C. The resulting surface integral of a curl [Eq. (31)] can be recast, using Stokes' theorem, into a contour integral and the last equality in Eq. (34) follows. Using the definition (12) of the dislocation current, Eq. (34) can be recast into a form that emphasizes the analogy with electromagnetism

$$\frac{1}{T}\int d^3x\,\sigma_{ik}(\mathbf{x})u_{ik}^C(\mathbf{x}) = i\int d^3x\,A_{lk}(\mathbf{x})j_l^C(\mathbf{x})b_k^C. \quad (35)$$

Changing the functional integration in Eq. (29) from σ to $\mathbf{h}$ and substituting Eqs. (33) and (35), we obtain

$$e^{-F_{el}[\mathbf{u}^{dis}]/T} = \int D\mathbf{h}\,e^{-F_0[\mathbf{h}]/T + i\int d^3x A_{lk}(\mathbf{x})\Sigma_C j_l^C(\mathbf{x})b_k^C}. \quad (36)$$

Notice that all the dependence on the coordinates of the dislocation loops is contained in the second term in exponent on the rhs of Eq. (36), which describes the deformation of the solid due to the presence of dislocations and accounts for all the interactions (both intra and interloop) between the segments of the dislocation loops. $F_0[\mathbf{h}]$ is the free energy associated with the usual thermal fluctuations of the solid (phonons) that are present even in the absence of dislocations. In the following we will use Eq. (36) to calculate the correlation function of dislocation charges.

The charge-charge correlation function $D_{ij\,kl}(\mathbf{x}-\mathbf{x}')$, Eq. (28), can be expressed as a response function to an external field $\mathbf{A}^{ext}$,

$$D_{ij\,kl}(\mathbf{x}-\mathbf{x}')=-\left.\frac{\delta^2 \ln Z[\mathbf{A}^{ext}]}{\delta A^{ext}_{ij}(\mathbf{x})\,\delta A^{ext}_{kl}(\mathbf{x}')}\right|_{\mathbf{A}^{ext}=0}, \tag{37}$$

where $Z[\mathbf{A}^{ext}]$ is obtained by replacing $\mathbf{A}\to\mathbf{A}+\mathbf{A}^{ext}$ in the Boltzmann weight, Eq. (36), and performing the trace over all the conformations of the loops

$$Z[\mathbf{A}^{ext}]\equiv\prod_{N\mathbf{b}}\frac{1}{n(N,\mathbf{b})!}\int D\mathbf{x} \times\int D\mathbf{h}e^{-F_0[\mathbf{h}]/T+i\int d^3x(A_{lk}+A^{ext}_{lk})\Sigma_C j^C_l b^C_k}. \tag{38}$$

Here, $n(N,\mathbf{b})$ is the number of dislocation loops with Burgers vector $\mathbf{b}$ and contour length aN, with a the size of a loop segment (the length of a bond in a lattice model of the solid) and N the number of segments. The functional integration $\int D\mathbf{x}$ is over the coordinates of the segments of the dislocation loops $\{C\}$.

We proceed to calculate the partition function in the presence of an infinitesimally small external field $\mathbf{A}^{ext}$. Changing the order of integration over $\mathbf{h}$ and over the loop coordinates we arrive at the following expression

$$Z[\mathbf{A}^{ext}]=\int D\mathbf{h}e^{-F_0[\mathbf{h}]/T}\prod_{N\mathbf{b}}\frac{(G_{N\mathbf{b}}[\mathbf{A}+\mathbf{A}^{ext}])^{n(N,\mathbf{b})}}{n(N,\mathbf{b})!} \tag{39}$$

where

$$G_{N\mathbf{b}}[\mathbf{A}+\mathbf{A}^{ext}]\equiv\int d^3x G_{N\mathbf{b}}(\mathbf{x},\mathbf{x}|\mathbf{A}+\mathbf{A}^{ext}). \tag{40}$$

The partition function $G_{N\mathbf{b}}(\mathbf{x},\mathbf{x}'|\mathbf{A})$ of a dislocation line of length N and Burgers vector $\mathbf{b}$ (with end points $\mathbf{x}$ and $\mathbf{x}'$), on a lattice with lattice constant a is calculated in Appendix A.

In the random phase approximation (RPA), the partition function of a dislocation is a Gaussian functional of $\mathbf{A}+\mathbf{A}^{ext}$ and the total partition function can be written in the form

$$Z[\mathbf{A}^{ext}]=\prod_{N\mathbf{b}}\frac{[VG^0_N(0)]^{n(N,\mathbf{b})}}{n(N,\mathbf{b})!}\int D\mathbf{h}e^{-F[\mathbf{h}]/T},$$

$$F[\mathbf{h}]=F_0[\mathbf{h}]+\frac{T}{2}\int d^3x\int d^3x' D^0_{kl\,k'l'}(\mathbf{x}-\mathbf{x}') \times[A_{kl}(\mathbf{x})+A^{ext}_{kl}(\mathbf{x})][A_{k'l'}(\mathbf{x}')+A^{ext}_{k'l'}(\mathbf{x}')], \tag{41}$$

where the partition function of a noninteracting loop, $G^0_N(0)$, is defined in Eq. (A4) of Appendix A. $D^0_{klk'l'}$ is the charge-charge correlation function of noninteracting dislocations ($\mathbf{A}=0$),

$$D^0_{kl\,k'l'}(\mathbf{x}-\mathbf{x}')=\sum_{N\mathbf{b}} n(N,\mathbf{b})b_l b_{l'} D^N_{k\,k'}(\mathbf{x}-\mathbf{x}'), \tag{42}$$

where $D^N_{k\,k'}$ can be interpreted as the current–current correlator of a noninteracting dislocation loop of N segments. The Fourier transform of this expression is calculated using Eqs. (37), (41), and (A9). We obtain

$$\tilde{D}^N_{k\,k'}(\mathbf{q})=\frac{1}{V}Q_{kk'}a^2Nd(a^2q^2N/8), \tag{43}$$

where

$$Q_{kk'}\equiv\delta_{kk'}-q_kq_{k'}/q^2 \tag{44}$$

is the transverse projection operator that satisfies $Q_{kk'}q_k=Q_{kk'}q_{k'}=0$, $Q_{kk'}Q_{k'l}=Q_{kl}$, and where

$$d(y)\equiv1+i\sqrt{\frac{\pi}{4y}}e^{-y}\,\mathrm{erf}(i\sqrt{y}), \tag{45}$$

with erf denoting the error function.

Substituting Eq. (43) into Eq. (42), we get

$$\tilde{D}^0_{klk'l'}(\mathbf{q})=\frac{a^2}{V}Q_{kk'}\sum_{N\mathbf{b}} n(N,\mathbf{b})Nb_lb_{l'}d(a^2q^2N/8). \tag{46}$$

For an isotropic distribution of Burgers vectors, $n(N,\mathbf{b})=n(N,b)$, this reduces to

$$\tilde{D}^0_{kl\,k'l'}(\mathbf{q})=D(q)Q_{kk'}\delta_{ll'},$$

$$D(q)=\frac{a^2}{3V}\sum_{N\mathbf{b}} n(N,b)Nb^2d(a^2q^2N/8). \tag{47}$$

In the long-wavelength limit $q\to0$, we get from Eq. (43)

$$D(q)=Dq^2,\quad D=\frac{a^4}{36V}\sum_{N\mathbf{b}} n(N,\mathbf{b})N^2b^2. \tag{48}$$

The vanishing of $D(q)$ in the limit $q\to0$, is a consequence of the relation $\int\mathbf{j}^C(\mathbf{x})d^3x=\oint ds(\partial\mathbf{x}/ds)=0$ [see Eq. (12)].

It is interesting to reflect on the physical meaning of the above results. Note that since $\mathbf{j}(\mathbf{x})=\oint ds(\partial\mathbf{x}/ds)\delta[\mathbf{x}(s)-\mathbf{x}]$ is the tangent to a dislocation loop at $\mathbf{x}$, $D^N_{kk'}(\mathbf{x}-\mathbf{x}')=\langle j_k(\mathbf{x})j_{k'}(\mathbf{x}')\rangle$ is the correlator of the tangent vectors at two points on the dislocation loop (of N segments), separated by spatial distance $|\mathbf{x}-\mathbf{x}'|$. A large noninteracting dislocation loop obeys the same Gaussian statistics as a polymer chain in theta solvent, where one expects such correlations to decay on length scales comparable with the persistence length a.[11] Fourier transforming the expression for $\tilde{D}^N_{kk'}(\mathbf{q})$, Eq. (43), we find that in the range $a\ll|\mathbf{x}-\mathbf{x}'|\ll aN^{1/2}$, the correlation is given by (this result was first derived in Ref. 12, in a study of interacting vortices in turbulent fluids)

$$\langle j_k(\mathbf{r})\, j_{k'}(0)\rangle \sim \left(\frac{3r_k r_{k'}}{r^5} - \frac{\delta_{kk'}}{r^3}\right). \tag{49}$$

Note that while the scalar product $\langle \mathbf{j}(\mathbf{r})\cdot\mathbf{j}(0)\rangle$ vanishes on length scales larger than the persistence length a, the correlation between different components of the tangent vector decays as a power law and is therefore quite long ranged. Since the only difference between our correlator and the one that appears in the usual calculation of the persistence length of Gaussian chains is the condition that the loop must pass through both points $\mathbf{x}$ and $\mathbf{x}'$, this imposes an unexpectedly strong constraint on the set of possible chain conformations. The conformations that make the dominant contribution to the correlator and lead to the appearance of long-range orientational correlations, are thus very different from the ones that dominate the ensemble of unconstrained Gaussian chains. Finally, as expected, the correlation decays exponentially on length scales larger than the Gaussian chain size, reflecting the fact that the probability to find two segments belonging to the same chain separated by distance larger than the average chain size, decreases exponentially with r^2/a^2N.[11]

We return to the calculation of the charge-charge correlator of interacting dislocation loops. The Gaussian path integral (41) can be calculated by introducing a shift of the integration variable $\tilde{h}_{ik}(\mathbf{q})\to\tilde{h}_{ik}(\mathbf{q})+\overline{h}_{ik}(\mathbf{q})$, where $\overline{h}_{ik}$ is found from the condition of equilibrium of the solid in a given external field $\mathbf{A}^{ext}$,

$$\frac{\delta F[\mathbf{h}]}{\delta\tilde{h}_{ik}(-\mathbf{q})}=0, \quad F[\mathbf{h}]\equiv VT\int\frac{d^3q}{(2\pi)^3}\tilde{f}(\mathbf{q}). \tag{50}$$

Here, $\tilde{f}(\mathbf{q})$ is the Fourier transform of the free-energy density

$$\tilde{f}(\mathbf{q})=\frac{q^4}{4\mu}\left[\tilde{h}_{ik}(\mathbf{q})\tilde{h}_{ik}(-\mathbf{q})-\frac{\nu}{1+\nu}\tilde{h}_{ll}(\mathbf{q})\tilde{h}_{jj}(-\mathbf{q})\right] + \frac{T}{2}D(q)Q_{kk'}[\tilde{A}_{kl}(\mathbf{q})+\tilde{A}^{ext}_{kl}(\mathbf{q})][\tilde{A}_{k'l}(-\mathbf{q}) + \tilde{A}^{ext}_{k'l}(-\mathbf{q})]+\lambda_i q_k[\tilde{h}_{ik}(-\mathbf{q})+\tilde{h}_{ki}(-\mathbf{q})] \tag{51}$$

and λ_i are Lagrange multipliers that enforce the ''Coulomb gauge'' constraint $q_k\tilde{h}_{ik}=q_k\tilde{h}_{ki}=0$.

Upon some algebra we obtain

$$\frac{q^2}{\mu}\left(\overline{h}_{ik}-\frac{\nu}{1+\nu}Q_{ik}\overline{h}_{ll}\right)+2\frac{D(q)}{T}\overline{h}_{ik} = -i\frac{D(q)}{Tq}(Q_{il}\tilde{A}^{ext}_{lj}C_{jk}+Q_{kl}\tilde{A}^{ext}_{lj}C_{ji}), \tag{52}$$

where $\tilde{\mathbf{A}}^{ext}$ is the Fourier transform of the function $\mathbf{A}^{ext}$ and C_{ij} is an antisymmetric tensor defined in Eq. (24). The solution of these equations can be simplified by noticing that the matrices $\mathbf{Q}$ and $\mathbf{C}$ have the following group properties under matrix multiplication

$$\mathbf{Q}^2=\mathbf{Q}, \quad \mathbf{Q}\cdot\mathbf{C}=\mathbf{C}\cdot\mathbf{Q}=\mathbf{C}, \quad \mathbf{C}^2=-\mathbf{Q}. \tag{53}$$

Taking the trace of Eq. (52) and using $Q_{ii}=2$ and $Q_{il}C_{ji}=C_{jl}$ we calculate the trace of $\overline{\mathbf{h}}$

$$\overline{h}_{ll}=-\frac{i}{q}\frac{2\mu D(q)/Tq^2}{1-\nu+2\mu(1+\nu)D(q)/Tq^2}. \tag{54}$$

Substituting this expression into Eq. (52), we get

$$\overline{h}_{ik}=-i\frac{R(q)}{q}[Q_{il}\tilde{A}^{ext}_{lj}C_{jk}+Q_{kl}\tilde{A}^{ext}_{lj}C_{ji}+S(q)Q_{ik}\tilde{A}^{ext}_{lj}C_{jl}],$$

$$R(q)\equiv\frac{\mu D(q)/T}{q^2+2\mu D(q)/T}, \tag{55}$$

$$S(q)\equiv\frac{2\nu}{1-\nu+2\mu(1+\nu)D(q)/Tq^2}.$$

Performing the Gaussian integral in Eq. (41) and using Eq. (37) we obtain the following expression for the charge-charge correlation function of interacting dislocation loops

$$\tilde{D}_{ij\,kl}(\mathbf{q})=D(q)\{Q_{ik}\delta_{jl}-R(q)\times[Q_{ik}Q_{jl}+C_{kj}C_{il}+S(q)C_{ij}C_{kl}]\}. \tag{56}$$

The first term in the curly brackets gives the contribution of noninteracting loops and the remaining terms [proportional to $R(q)$] describe the ''polarization'' of the elastic medium due to the interaction between the segments of dislocation loops. An alternative interpretation is to view the interaction between the dislocation loops as mediated by phonons. In this language, R represents the contribution of transverse phonons and S that of longitudinal phonons. Since $q_i\tilde{D}_{ij\,kl}=q_k\tilde{D}_{ij\,kl}=0$, only transverse phonons couple directly to the charge-charge correlator, and longitudinal phonons contribute only indirectly, through their coupling with the transverse ones [the RS term in Eq. (56)]. The appearance of D in the denominators of R and S can be interpreted as a renormalization effect, which reduces the effective interaction between the dislocations. Note that the polarization correction vanishes in the limit $q\to\infty$ and therefore does not affect the small-scale behavior of the charge-charge correlation function which is given by its bare value $\tilde{D}^0_{ij\,kl}(\mathbf{q})$.

Dislocation-induced corrections to the elastic moduli of an isotropic solid have the following tensorial structure

$$\frac{1}{V}\langle U^{dis}_{ij}U^{dis}_{kl}\rangle=A_1(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk})-A_2\delta_{ij}\delta_{kl}. \tag{57}$$

The scalar functions

$$A_i=\frac{D}{1+2\mu D/T}\left[\alpha_i(\nu)-\frac{2\nu\beta_i(\nu)\mu D/T}{1-\nu+2(1+\nu)\mu D/T}\right], \tag{58}$$

were calculated in Appendix B [explicit expressions for the coefficients $\alpha_i(\nu)$ and $\beta_i(\nu)$ are given in Eq. (B9)]. The renormalized elastic moduli are obtained by inserting the expressions in Eqs. (57), (58), and (20) into Eq. (19)

$$\frac{1}{4\mu_R}=\frac{1}{4\mu}+\frac{A_1}{T} \tag{59}$$

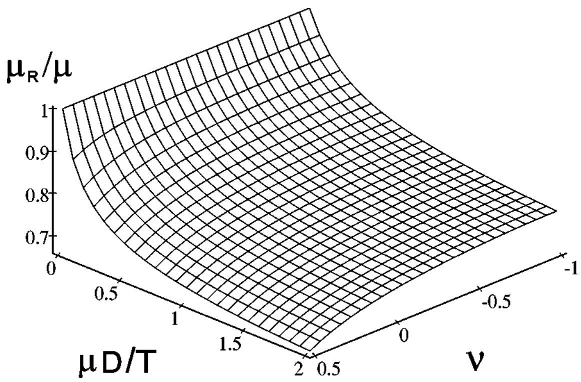

FIG. 1. A three-dimensional plot of the renormalized shear modulus μ_R/μ as a function of the bare Poisson ratio ν and the dimensionless parameter $\mu D/T$.

$$\frac{1}{4\mu_R}\frac{2\nu_R}{1+\nu_R}=\frac{1}{4\mu}\frac{2\nu}{1+\nu}+\frac{A_2}{T}. \tag{60}$$

In Fig. 1, we present a $3d$ plot of the scaled renormalized shear modulus, μ_R/μ, as a function of $\mu D/T$ and ν. We find that the modulus is a monotonically decreasing function of the concentration and size of dislocation loops and that it approaches a finite limit when the average loop size diverges $(D\to\infty)$. This statement is valid as long as the size of the loops is smaller than the size of the sample. It is interesting to note that a qualitatively similar behavior of the shear modulus was predicted in the low-temperature phase of $2d$ solids.[2]

In Fig. 2 we plot the renormalized vs the bare Poisson ratio of the solid, in the limit $D\to\infty$ (the effect of dislocations is maximized in this limit). As expected, there is no renormalization of the bare Poisson ratio of an incompressible ($\nu=\frac{1}{2}$) or an unstable ($\nu=-1$) solid and the renormalization is rather small for intermediate values of ν. The presence of dislocations increases the Poisson ratio when the bare ratio is in the range $\sim 0.2-0.5$ and decreases it for smaller values of ν.

The observation that the shear modulus remains finite in the presence of a finite concentration of dislocation loops of arbitrary finite size, deserves some explanation. The renormalization of the elastic moduli is determined by the long-wavelength $(q\to 0)$ limit of the charge-charge correlation function $\tilde{D}_{ij\,kl}(\mathbf{q})$, with $D(q)=Dq^2$ [Eq. (48)] and $R(q)$ and $S(q)$ approaching constant values [Eq. (55)]. Since D diverges with increasing loop size [see Eq. (48)], strong renormalization of the elastic moduli is expected. This is prevented by the appearance of D in the denominators of $R(q)$ and $S(q)$, which suppresses the phonon-mediated long-range interactions between the loops.

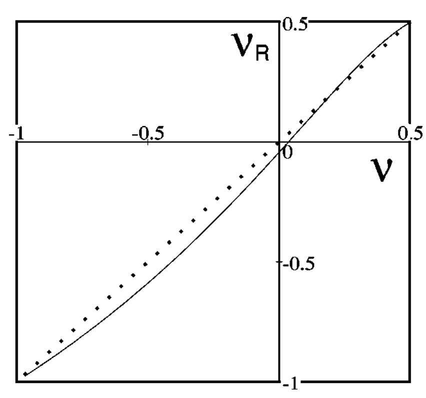

FIG. 2. Plot of the renormalized Poisson ratio ν_R as a function of the bare Poisson ratio ν, for $\mu D/T\to\infty$. The dotted $\nu_R=\nu$ line is drawn for comparison.

Does this mean that there is no dislocation-induced melting transition in $3d$? A careful examination of the above argument shows that it breaks down if ''open'' dislocation lines that terminate on the boundaries of the solid, appear in the system. For example, let us consider the force on a dislocation with contour Γ, due to constant stress σ inside the solid

$$\mathbf{f}=\int_\Gamma d\mathbf{x}\times(\sigma\cdot\mathbf{b}). \tag{61}$$

This expression vanishes for closed loops but remains finite for open lines and since the force on a dislocation must vanish in equilibrium, we conclude that the stress must vanish inside the sample. This also means that in the presence of open infinite dislocation lines, shear stress applied to the surface does not penetrate into the bulk of the sample and therefore the system behaves as a (nonviscous) fluid. This screening of the stress is analogous to the expulsion of the magnetic field by a superconductor (Meissner effect[13]).

Although this simple mechanical argument does not account for the statistical nature of the problem, the conclusion that the system behaves as a liquid in the presence of infinite dislocation lines, remains valid even when fluctuations are taken into consideration. The presence of such $N\to\infty$ lines leads to the screening of interactions between dislocations on length scales larger than a screening length and is characteristic of the ''confining'' phase[14] in which there are no free-transverse phonons. The magnitude of this screening length can be estimated as follows. Differentiating twice the dislocation line energy, Eq. (A14) [Appendix (A)], with respect to $\tilde{\mathbf{A}}$ we obtain the following RPA expression for the current-current correlator, valid for all $qa\ll 1$,

$$\tilde{D}^N_{ik}(q)=\frac{a^2N}{V}Q_{ik}. \tag{62}$$

Fourier transforming Q_{ik} back to coordinate space gives the current-current correlator of a noninteracting loop, Eq. (49). The identity of the correlators follows from the observation that, on length scales smaller than loop size, the segments do not ''know'' whether they belong to a finite loop or to an infinite line. Equation (62) gives a q-independent $D(q)\simeq a\phi/3$ where ϕ is the volume fraction occupied by the dislocation lines (we assumed that the distribution of Burgers vectors is isotropic and replaced the Burgers vector by its minimal value $\sim a$). The screening length λ is obtained by substituting this constant into the expression for $R(q)$, Eq. (55), and demanding that the two terms in the denominator of $R(q)$ be equal for $q=1/\lambda$. This yields

$$\lambda=\frac{1}{\sqrt{2\mu D(q)/T}}\simeq a\sqrt{\frac{T}{\mu a^3\phi}}, \tag{63}$$

In the presence of such strong screening, different dislocation lines contribute independently to the correlator $\langle U_{ij}^{dis}U_{kl}^{dis}\rangle$. Since the characteristic displacement associated with a dislocation line is of order b, integrating over the surface of the solid, Eq. (18), yields $U^{dis}\sim L^2 b$, where L is the size of the system (we omit tensor indices in this simple scaling estimate). The dislocation correction to the inverse elastic modulus, Eq. (19), scales as

$$\frac{1}{V}\langle U^{dis}U^{dis}\rangle\sim\frac{1}{L^3}n(L^2b)^2\sim\phi L^2, \tag{64}$$

where $n\sim\phi L^3/N$ is the number of dislocation lines and we have used the free Gaussian chain relation, $N\sim L^2$. The divergence of this correction with system size shows that the modulus is renormalized to zero when a nonvanishing concentration of infinite dislocation lines appears in the system. This conforms with the intuitive expectation that the system can not sustain shear in the presence of such dislocation lines and should be considered as a liquid. Note, however, that in real solids the motion of dislocations may be hampered by the presence of kinetic barriers and solidlike response to stress on experimentally relevant time scales may result even in the presence of infinite dislocation lines.[8]

V. EQUILIBRIUM DISTRIBUTION OF DISLOCATIONS

Up to this point we have assumed that the distribution of dislocation loops is fixed, i.e., that dislocations are created by some irreversible method and that they can no longer be created or annihilated later on. The rationale behind this approach is that since the core energy per bond in a typical solid is of the order of few electron volts (far in excess of the thermal energy k_BT), the probability of creating a dislocation loop by a thermal fluctuation is exponentially small[8] and dislocations are nonequilibrium entities. With this assumption there is a close analogy between the statistical physics of dislocation loops and that of polymer molecules, the chemical structure of which is assumed to be fixed and only the conformational degrees of freedom are taken into consideration. The main simplification compared to the polymer case is the fact that dislocations can pass freely through each other and therefore topological entanglements play no role in the conformational statistics of dislocation loops.

Despite the fact that dislocations in most solids are not of thermal origin, in this section we will follow the path of our predecessors[4–7] and consider the free energy and the equilibrium distribution of dislocations. While this can be viewed as an formal exercise in equilibrium statistical mechanics, there is a possibility that such a scenario can be realized in intermediate phases of some ''soft'' solids. Potential candidates are the so-called ''rotator'' phases of normal alkanes,[15] in which shear moduli are at least two orders of magnitude smaller than in the low-temperature crystalline phase.[16]

Assuming that dislocations reach thermal equilibrium with respect to their loop sizes and Burgers vectors (this is possible only if the core energy per segment is not much larger then k_BT), the equilibrium value of $n(N,b)$ is obtained by minimizing the free energy, $F=-T\ln Z$, where the partition function of the system of interacting dislocations is defined in Eq. (41). To eliminate the divergence of the Gaussian integrals in Eq. (41), we introduce a cutoff at wave vector $q_0\gtrsim 1/a$ and add core energy $E_b(q_0)$ per segment of a dislocation loop with Burgers vector b, to the free energy. This core energy accounts for interactions between loop segments separated by spatial distances smaller than $1/q_0$. We arrive at the following expression for the excess free energy in the presence of dislocations with a given distribution $n(N,b)$

$$F=\sum_{N\mathbf{b}}n(N,b)\left[T\ln\frac{n(N,b)}{eVG_N^0(0)}+E_b(q_0)N\right]$$
$$+VT\int_{|q|<q_0}\frac{d^3q}{(2\pi)^3}\left\{\ln\left[1+\frac{2\mu D(q)}{Tq^2}\right.\right.$$
$$\left.\left.+\frac{1}{2}\ln\left[1+\frac{2\mu D(q)}{Tq^2}\,\frac{1+\nu}{1-\nu}\right]\right]\right\}, \tag{65}$$

where the function $D(q)$ is defined in Eq. (47). The first logarithmic term describes the translational and conformational entropy of the loops. The two logarithmic terms under the integral account for both the intra and the interloop interactions between the dislocations.

Minimizing the above free energy subject to the relation between $D(q)$ and $n(N,b)$, Eq. (47), and substituting the expression for $G_N^0(0)$, Eq. (A4), we find the equilibrium value of $n(N,b)$

$$n_{eq}(N,b;T)=\frac{Vz^N}{(2\pi a^2N)^{3/2}}e^{-E_b^RN/T}, \tag{66}$$

where z is the coordination numberr of the lattice and

$$E_b^R=E_b(q_0)+\frac{\mu a^2b^2q_0}{9\pi^2}\left\{\frac{3-\nu}{1-\nu}-C_\nu\left[\frac{2\mu D(q_0)}{Tq_0^2}\right]^{1/2}\right\},$$
$$C_\nu\equiv 2+\left(\frac{1+\nu}{1-\nu}\right)^{3/2} \tag{67}$$

can be regarded as a renormalized core energy. In deriving Eqs. (66) and (67), we used the approximation $\mu D(q_0)/Tq_0^2\ll 1$, which is equivalent to the condition of validity of the RPA.

Following the renormalization group approach,[10] we define the ''bare'' core energy E_b^{bare} into which we adsorb all the details of the small-scale behavior

$$E_b(q_0)=E_b^{bare}-\frac{\mu a^2b^2q_0}{9\pi^2}\,\frac{3-\nu}{1-\nu}. \tag{68}$$

Substituting Eq. (68) into Eq. (67), we get

$$E_b^R=E_b^{bare}-C_\nu\frac{\mu a^2b^2}{9\pi^2}\left[2\frac{\mu}{T}D(q_0)\right]^{1/2}. \tag{69}$$

The energy $E_b^{bare}\simeq\mu ab^2$ accounts for deviations from the linear theory of elasticity in the strongly deformed region associated with the core of a dislocation, and does not depend on the distribution $\{n(N,b)\}$. The second term on the rhs of Eq. (69) gives the contribution of effective interactions between non-neighboring segments of a loop, that can be described in the framework of the linear theory of elasticity. Although the interaction between the segments can be repulsive or attractive depending on their relative orientation and the direction of the Burgers vector, configurations in which the interaction is attractive will have a larger Boltzmann weight and the resulting effective interaction will be attractive, thus reducing the core energy, Eq. (69). Note that within the domain of validity of the RPA, corrections to the bare core energy due to fluctuation-induced attractions between segments of loops are small and therefore E_b^R is of order E_b^{bare}.

Using the same renormalization procedure for the free energy, Eq. (65), we find

$$F=\sum_{N\mathbf{b}} n(N,b)\left[T\ln\frac{n(N,b)}{eVG_N^0(0)}+E_b^{bare}N\right] - C_\nu\frac{VT}{6\pi^2}\left[2\frac{\mu}{T}D(q_0)\right]^{3/2}, \tag{70}$$

where the last term is due to fluctuation corrections which reduce the free energy.

Substituting Eq. (66) into Eq. (48) we obtain a closed-form equation for the parameter $D(q_0)$ (which does not depend on the cutoff q_0)

$$D(q_0)=\frac{a^2}{3V}\sum_{N\mathbf{b}} n_{eq}(N,b;T)Nb^2. \tag{71}$$

Inserting this expression into Eq. (70) we find that the fluctuation correction to the free energy scales with the $\frac{3}{2}$ power of the concentration of dislocation segments, in agreement with the result of Edwards and Warner.[4] In principle, one can use the thermodynamic free energy, Eq. (70), to study the dislocation-induced melting transition. This was done in Ref. 4 and will not be repeated here. Instead, we will go beyond the random phase approximation and study the hitherto neglected effect of fluctuation-induced attractions on the conformation of dislocation loops.

VI. FLUCTUATION EFFECTS ON LOOP CONFORMATION

In the preceding sections we used the random phase approximation (assuming Gaussian statistics of dislocation loops) and found that this approximation is selfconsistent in the parameter range

$$\frac{\mu a^2}{T}D(q_0)=\frac{\mu a^4}{3TV}\sum_{N\mathbf{b}} n_{eq}(N,b;T)Nb^2\ll 1, \tag{72}$$

which can be interpreted as the Ginsburg criterion[10] for our system. Defining the average volume fraction of loop segments as ϕ and assuming that only the smallest Burgers vectors ($b\simeq a$) contribute to the sum, this criterion can be rewritten as

$$\frac{\mu a^3}{T}\phi\ll 1, \quad \phi\equiv\frac{a^3}{V}\sum_N n_{eq}(N;T)N, \tag{73}$$

which states that the average interaction energy between dislocation segments is much smaller than the thermal energy. Since for most solids $\mu a^3 \gg T$ throughout the physical range of parameters, RPA applies only at very small dislocation densities.

Inspection of Eq. (73) shows that, for a given concentration of dislocations, the RPA breaks down at sufficiently low temperatures. The situation is reversed in equilibrium (with respect to formation and annihilation of dislocations), since the equilibrium concentration of dislocations increases exponentially with temperature [see Eq. (66)]. The breakdown of RPA occurs when fluctuation-induced attractions between segments overcome the conformational entropy of the loops, and the random walk configurations of large loops are replaced by more compact ones. The physical origin of this effective attraction was discussed in the preceding section: while the interaction between loop segments may be either attractive or repulsive, depending on the relative orientation of their directors (tangents to the loops), Burgers vectors and relative separation, conformations in which intersegment attractions dominate have a higher Boltzmann weight and occur more frequently in the process of thermodynamic fluctuations. In this section, we use a variational approach to study the change of conformational statistics of the loops produced by this effective attraction. In Appendix C we present a perturbative analysis of the effect of intersegment attractions on the radii of gyration of dislocation loops and show that the results are in good agreement with those of the variational calculation.

We begin with the exact expression for the partition function of a loop in the presence of a ''potential'' (tensor) field $\mathbf{A}(\mathbf{x})$ [see Appendix (A)],

$$G_{N\mathbf{b}}[\mathbf{A}]=\oint D\mathbf{x}\exp\left\{-\frac{1}{2a^2}\int_0^N\left(\frac{\partial\mathbf{x}}{\partial s}\right)^2 ds - i\oint d\mathbf{x}(s)\cdot\mathbf{A}[\mathbf{x}(s)]\cdot\mathbf{b}\right\} \equiv \oint D\mathbf{x}\exp(-H[\mathbf{x}|\mathbf{A}]), \tag{74}$$

where the second equality defines the effective Hamiltonian H. We approximate this partition function by the following trial function

$$G_{N\mathbf{b}}^{tr}[\mathbf{A}]=\oint D\mathbf{x}\exp\left[-\sum_i\frac{1}{2a_i^2}\int_0^N\left(\frac{\partial x_i}{\partial s}\right)^2 ds\right] \times\left\{1-i\oint d\mathbf{x}(s)\cdot\mathbf{A}[\mathbf{x}(s)]\cdot\mathbf{b}\right\} \equiv\oint D\mathbf{x}\exp(-H^{tr}[\mathbf{x}|\mathbf{A}]). \tag{75}$$

The trial Hamiltonian H^{tr} is defined by the second equality. The renormalized statistical segment lengths a_i depend on the potential field and will be determined selfconsistently later on. Because of the mean-field character of our variational procedure the loop dimensions are those of an anisotropic Gaussian random walk, i.e., $\langle R_i^2\rangle^{tr}=a_i^2 N$ along the i axis ($\{i\}=x,y,z$).

To calculate the partition function (74) we use the following variational principle[10]

$$\ln G_{N\mathbf{b}}[\mathbf{A}]\geqslant \ln G_{N\mathbf{b}}^{tr}[\mathbf{A}]-\langle H[\mathbf{x}|\mathbf{A}]-H^{tr}[\mathbf{x}|\mathbf{A}]\rangle_{tr}, \quad (76)$$

where the averaging is taken with the trial Hamiltonian Eq. (75). We will use the right-hand side of Eq. (76) as an approximation to the exact $\ln G_{N\mathbf{b}}$, with parameters a_i, which minimize the free energy. Expanding it to the second order in **A** we get (see Appendix A)

$$\ln G_{N\mathbf{b}}[\mathbf{A}]\simeq \ln VG_N(0)-\sum_i \left[\ln\frac{a_i}{a}+\frac{1}{2}-\frac{1}{2}\left(\frac{a_i}{a}\right)^2\right]$$
$$-\frac{(a^R)^2N}{2V}\int\frac{d^3q}{(2\pi)^3}d\left[\frac{(a^R)^2q^2N}{8}\right]$$
$$\times Q_{nm}b_l b_k\tilde{A}_{nl}(\mathbf{q})\tilde{A}_{mk}(-\mathbf{q}), \quad (77)$$

with $(a^R)^2=\frac{1}{3}\Sigma_i a_i^2$.

We shall not repeat the derivation of the free energy and show only the final expression

$$F=\sum_{N\mathbf{b}} n(N,b)\left\{T\ln\frac{n(N,b)}{eVG_N^0(0)}+E_b^{bare}N\right.$$
$$\left.+T\sum_i\left[\ln\lambda_i^{N\mathbf{b}}+\frac{1}{2}-\frac{1}{2}(\lambda_i^{N\mathbf{b}})^2\right]\right\}$$
$$-C_\nu\frac{VT}{6\pi^2}\left[2\frac{\mu}{T}D_{var}(q_0)\right]^{3/2}, \quad (78)$$

where $\lambda_i^{N\mathbf{b}}\equiv a_i^{N\mathbf{b}}/a=\langle(R_i^{N\mathbf{b}})^2\rangle^{1/2}/(aN^{1/2})$ are the compression coefficients of a loop of N segments and Burgers vector **b** and

$$D_{var}(q_0)=\frac{a^2}{3V}\sum_{N\mathbf{b}}\frac{1}{3}\sum_i(\lambda_i^{N\mathbf{b}})^2 n(N,b)Nb^2. \quad (79)$$

Note that the RPA corresponds to the choice $\lambda_i^{N\mathbf{b}}=1$. Here, we determine these coefficients from the condition that they minimize the free energy Eq. (78)

$$\frac{1}{(\lambda^{Nb})^2}=1+C_\nu\frac{\mu a^2b^2N}{9\pi^2T}\left[2\frac{\mu}{T}D_{var}(q_0)\right]^{1/2}, \quad (80)$$

where C_ν is defined in Eq. (67) and $\lambda_i^{N\mathbf{b}}=\lambda^{Nb}$. This expression agrees (within few percent) with the perturbative result in Appendix C.

Since $\lambda^{Nb}<1$, we conclude that fluctuation-induced attraction between segments leads to isotropic compression of the radii of gyration of the loops compared to their unperturbed Gaussian dimensions. Within our approximation, the compression increases with loop size and with average concentration of dislocations. One can easily show, using Eq. (80), that the condition of validity of the variational theory becomes

$$2\frac{\mu a^2}{T}D_{var}(q_0)=\left\{\frac{6\pi^2a^3}{C_\nu V}\sum_{N\mathbf{b}} n(N,b)[1-(\lambda^{Nb})^2]\right\}^{2/3}\ll 1. \quad (81)$$

Note that unlike the criterion for the validity of the RPA, which involves the density of segments, the above criterion for the validity of the variational approach involves the far smaller density of loops and therefore has a much broader domain of applicability.

The renormalized elastic moduli are defined by Eqs. (59) and (60), where the coefficients A_i are given by Eqs. (58) with the substitution

$$D\to D_{var}=\frac{a^4}{36V}\sum_{N\mathbf{b}}(\lambda^{Nb})^4 n(N,\mathbf{b})N^2b^2. \quad (82)$$

Since the renormalized shear modulus μ_R is a monotonically decreasing function of D, we conclude that the RPA overestimates the dislocation-induced suppression of the shear modulus. Although our variational estimate is by no means exact, it suggests that fluctuations tend to reduce the effect of the dislocations on the elastic constants of the solid. Note that Fig. 1 remains unchanged provided we replace the variable $\mu D/T$ by $\mu D_{var}/T$.

VII. DISCUSSION

In this paper, we studied the physics of interacting dislocation loops and their effect on the elastic moduli of isotropic solids. We found that while the Poisson ratio can either increase or decrease in the presence of dislocations depending on its ''bare'' value, the shear modulus decreases monotonically to a finite limiting value with increasing concentration and size of the loops. The conclusion that an arbitrary concentration of finite dislocation loops in a solid has a relatively minor effect on the elastic moduli is quite unexpected. Inspection of the derivation shows that this is a consequence of the fact that the renormalization of the moduli depends on the interplay of two opposing effects: while the introduction of additional dislocations increases the correlations between the ''charges,'' it also enhances the screening of their interactions. These two effects largely cancel each other and, therefore, within the limits of validity of our model, the shear modulus does not vanish when the concentation of finite loops increases.

Even though the physics of topological defects appears to be very different in 2 and in $3d$, our prediction that the shear modulus vanishes and the solid undergoes dislocation-induced melting only when infinite dislocation lines appear in the sample, agrees with that of Ref. 2 for $2d$ solids. In the final analysis, the physics of fluctuating loops may be not very different from that of that of vortices; due to the long-range vectorial correlations between segments of a dislocation loop, its partition function is dominated by configurations in which the forces between the segments are predominantly attractive and, in this sense, a single dislocation loop resembles a vortex-antivortex pair. Furthermore, while there is no vortex unbinding transition in $3d$, both the Kosterlitz-Thouless transition in $2d$ and the appearance of infinite dislocation lines in $3d$, are closely related to the screening of interactions between topological defects.

Are our results relevant to real solids? In principle, one could prepare solids with different concentrations of dislocations and study their response to small applied deformation. As long as the dimensionless parameter $\mu D/T \simeq(\mu a^3/T)\phi\overline{N}$ is much smaller then unity (ϕ is the volume fraction of sites occupied by dislocation loops and $\overline{N}$ is the average loop size), we predict that the shear modulus is not affected by the presence of dislocations. Indeed, while dislocations are known to control the response of solids to large applied stresses and account for plastic flow and limiting strength of materials,[17] they have little effect on the shear modulus, which determines the response to infinitesimal stresses.[18] We expect the renormalization of the shear modulus to become significant only when the above dimensionless parameter becomes of order unity. The prospects for experimental observation of this phenomenon are unclear because of the difficulty of controlling the distribution of dislocations.

Another issue that should be kept in mind when considering the application of our results to real solids is that of time scales. Experimental studies of the response of the solid to external perturbations on time scales smaller than that on which rearrangement and deformation of dislocation loops takes place (e.g., instantaneous measurement of stress following step strain), measure the ''adiabatic'' (bare) modulus μ. In order to measure the ''isothermal'' (renormalized) shear modulus μ_R one has to monitor the elastic response on time scales longer than the relaxation times associated with the kinetics of dislocations. Whether such time scales are experimentally accessible or not, depends on the temperature and on the height of the corresponding kinetic barriers.[17] Consideration of such issues is outside the scope of the present work.

We would like to discuss our model assumptions regarding the distribution of dislocations in a solid. Application of the methods of equilibrium statistical physics to the problem of topological defects in $3d$ crystalline solids is somewhat artificial in view of the fact that the core energies of these defects are normally much higher than thermal energies and therefore there should be almost no dislocations in a solid in true thermal equilibrium. In this paper we assumed that a given distribution of dislocations was produced by some nonequilibrium process such as nonequilibrium crystal growth or application of large stresses to the sample. Although we allowed the dislocation loops to move and change their conformation in the process of thermal fluctuations, we did not consider the higher energy (and therefore less probable) events of creation and annihilation of dislocation loops and changes of their contour length. While plausible, these model assumptions were motivated mainly by considerations of simplicity and the wish to maintain as close an analogy as possible with polymer physics, in order to benefit from the well-developed theoretical tools in this field.

In order to decide what kind of systems are the best candidates for observing some of the phenomena predicted by our theory, one has to ask the following question: in what type of solids is the energy of topological defects sufficiently low for thermal effects to play an important role? Since dislocations can be easily created on the surface of a crystal, they are expected to affect the physical properties of small particles and it is possible that they play a role in the observed surface melting of nanocrystals.[19] Equilibrium defects can arise in soft solids such as, for example, rotator phases of alkanes[16] and colloidal crystals. More exotic candidates are amorphous solids and glasses in which disclinations of an unusual type (Rivier lines[20]) are possible. Since the underlying symmetry is that of rotations in $3d$, a field-theoretical description of these topological defects involves a Yang-Mills-type theory of non-Abelian gauge fields[20] and its physical consequences remain to be elucidated.

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APPENDIX A: PARTITION FUNCTION OF DISLOCATIONS

1. Finite loops

We calculate the partition function of a dislocation loop of N segments (of length a each) and Burgers vector $\mathbf{b}$, placed on a lattice with lattice constant a. We find the following recurrence relation

$$G_{N+1\mathbf{b}}[\mathbf{x},\mathbf{x}'|\mathbf{A}]=\sum_{\mathbf{a}} e^{-i\mathbf{a}\cdot\mathbf{A}(\mathbf{x})\cdot\mathbf{b}}G_{N\mathbf{b}}[\mathbf{x}+\mathbf{a},\mathbf{x}'|\mathbf{A}]$$

$$=\sum_{\mathbf{a}} e^{\mathbf{a}\cdot[\boldsymbol{\nabla}-i\mathbf{A}(\mathbf{x})\cdot\mathbf{b}]}G_{N\mathbf{b}}[\mathbf{x},\mathbf{x}'|\mathbf{A}], \quad \text{(A1)}$$

where $\mathbf{A}\cdot\mathbf{b}$ is a vector with components $A_{ij}b_j$ and the summation is over z nearest neighbors on the lattice. In the continuum limit, Eq. (A1) reduces to the following differential equation for the partition function

$$\left[\frac{\partial}{\partial N}-\ln z-\frac{a^2}{2}(\nabla-i\mathbf{A}\cdot\mathbf{b})^2\right]G_{N\mathbf{b}}[\mathbf{x},\mathbf{x}'|\mathbf{A}]=0, \quad \text{(A2)}$$

with the initial condition

$$\lim_{N\to 0} G_{N\mathbf{b}}[\mathbf{x},\mathbf{x}'|\mathbf{A}]=\delta(\mathbf{x}-\mathbf{x}'). \quad \text{(A3)}$$

The solution for $\mathbf{A}=0$ is well known in polymer physics,[11]

$$G_N^0(\mathbf{x}-\mathbf{x}')=\frac{z^N}{(2\pi a^2N)^{3/2}}\exp\left[-\frac{(\mathbf{x}-\mathbf{x}')^2}{2a^2N}\right]. \quad \text{(A4)}$$

In order to obtain the solution for $\mathbf{A}\neq 0$ we notice that Eq. (A2) can be recast into the following integrodifferential equation

$$G_{N\mathbf{b}}[\mathbf{x},\mathbf{x}'|\mathbf{A}]=G_N^0[\mathbf{x}-\mathbf{x}']-\frac{a^2}{2}\int_0^N dN'\int d^3y\, G^0_{N-N'}(\mathbf{x}-\mathbf{y})$$

$$\times\{2iA_{ij}(\mathbf{y})b_j\nabla_i+i[\nabla_iA_{ij}(\mathbf{y})]b_j$$

$$+A_{ij}(\mathbf{y})A_{ik}(\mathbf{y})b_jb_k\}G_{N'\mathbf{b}}[\mathbf{y},\mathbf{x}'|\mathbf{A}]. \quad \text{(A5)}$$

This equation can be solved perturbatively by expanding the right-hand side to second order in $\mathbf{A}$. We then Fourier transform A_{ij} (the corresponding Fourier components are denoted by $\tilde{A}_{ij}$), set $\mathbf{x}=\mathbf{x}'$ and integrate over $\mathbf{x}$ using the Feynman-Kac relation

$$\int d^3x G^0_{N-N'}(\mathbf{x}_1-\mathbf{x})G^0_{N'}(\mathbf{x}-\mathbf{x}_2)=G^0_N(\mathbf{x}_1-\mathbf{x}_2) \quad \text{(A6)}$$

and the integral relation (valid for an arbitrary function f)

$$\int_0^N dN'\int_0^{N'} dN''f(N'')=\int_0^N ds(N-s)f(s). \quad \text{(A7)}$$

Since we want to calculate the contribution of the loop partition function to the free energy, we take the logarithm of both sides of Eq. (A5) and, expanding the logarithm to order $\mathbf{A}^2$ we obtain

$$\ln\frac{1}{VG^0_N(0)}\int d^3xG_{N\mathbf{b}}[\mathbf{x},\mathbf{x}|\mathbf{A}]$$
$$=-\frac{a^2}{2V}\int\frac{d^3q}{(2\pi)^3}\tilde{A}_{nl}(\mathbf{q})\tilde{A}_{mk}(-\mathbf{q})b_lb_k$$
$$\times\left\{\delta_{nm}N-\frac{a^2}{2G^0_N(0)}\int_0^N ds(N-s)\int d^3xe^{i\mathbf{q}\cdot\mathbf{x}}\right.$$
$$\left.\times\left(iq_n-\frac{2x_n}{a^2s}\right)\left[iq_m-\frac{2x_m}{a^2(N-s)}\right]G^0_s(\mathbf{x})G^0_{N-s}(\mathbf{x})\right\}. \quad \text{(A8)}$$

Calculating the integrals over $\mathbf{x}$ and s, we get

$$\ln\frac{G_{N\mathbf{b}}[\mathbf{A}]}{VG^0_N(0)}=-\frac{a^2N}{2V}\int\frac{d^3q}{(2\pi)^3}d\left(\frac{a^2q^2N}{8}\right)$$
$$\times Q_{nm}b_lb_k\tilde{A}_{nl}(\mathbf{q})\tilde{A}_{mk}(-\mathbf{q}), \quad \text{(A9)}$$

where $d(y)\equiv 1+i\sqrt{\pi/4y}e^{-y}\,\mathrm{erf}(i\sqrt{y})$ and erf is the error function. Q_{nm} is the transverse projection operator defined in Eq. (44).

2. Infinite lines

The general solution of Eq. (A2) for the partition function of a dislocation line with ends at points $\mathbf{x}$ and $\mathbf{x}'$ can be represented in the form

$$G_{N\mathbf{b}}[\mathbf{x},\mathbf{x}'|\mathbf{A}]=z^N\sum_r \psi^*_r(\mathbf{x})\psi_r(\mathbf{x}')e^{-\epsilon_rN}, \quad \text{(A10)}$$

where $\psi_r(\mathbf{x})$ are the normalized solutions of the eigenvalue equation

$$-\frac{a^2}{2}(\nabla-i\mathbf{A}\cdot\mathbf{b})^2\psi_r(\mathbf{x})=\epsilon_{\alpha r}\psi_r(\mathbf{x}),$$
$$\int \psi^*_r(\mathbf{x})\psi_s(\mathbf{x})d^3x=\delta_{rs}. \quad \text{(A11)}$$

For lines of infinite length, $N\to\infty$, only the ground state $r=0$ contributes to the sum in Eq. (A10).

The partition function of an infinite dislocation line with end points on the surface of the solid $G_{\mathbf{b}}[\mathbf{A}]$, can be obtained by integrating over the surface coordinates of both ends. Up to $1/N$ corrections this gives

$$\ln G_{\mathbf{b}}[\mathbf{A}]\equiv N\ln z-N\epsilon_0[\mathbf{A}]. \quad \text{(A12)}$$

Note that the eigenvalue $\epsilon_0[\mathbf{A}]$ can be found from the variational principle

$$\epsilon_0[\mathbf{A}]=\min_{\psi_0}\int d^3x\frac{a^2}{2}|(\nabla-i\mathbf{A}\cdot\mathbf{b})\psi_0|^2, \quad \int d^3x|\psi_0|^2=1. \quad \text{(A13)}$$

Expanding this function in powers of $\mathbf{A}$ we find the energy of an infinite line with finite density N/V of occupied bonds

$$\epsilon_0[\mathbf{A}]=\frac{a^2N}{2V}\int\frac{d^3q}{(2\pi)^3}Q_{nm}b_lb_k\tilde{A}_{nl}(\mathbf{q})\tilde{A}_{mk}(-\mathbf{q}). \quad \text{(A14)}$$

APPENDIX B: CALCULATION OF RENORMALIZED MODULI

In an isotropic homogeneous medium the correlator $\langle U^{dis}_{ij}U^{dis}_{kl}\rangle$ defining the renormalization of elastic moduli tensor (19) has the following tensor structure

$$\frac{1}{V}\langle U^{dis}_{ij}U^{dis}_{kl}\rangle=A_1(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk})-A_2\delta_{ij}\delta_{kl}. \quad \text{(B1)}$$

To find the constants A_i we consider different contractions of the tensor (B1)

$$I\equiv\frac{1}{V}\langle U^{dis}_{ii}U^{dis}_{kk}\rangle=6A_1-9A_2$$

$$J\equiv\frac{1}{V}\langle U^{dis}_{ij}U^{dis}_{ij}\rangle=12A_1-3A_2$$

in terms of which A_i can be expressed as

$$A_1=(3J-I)/30, \quad A_2=(J-2I)/15. \quad \text{(B2)}$$

We now proceed to calculate I and J.

We begin with the calculation of J by substituting Eqs. (23) and (56) into (27)

$$\Xi_{ijij}(\mathbf{q})=\left(\delta_{ij'}C_{ji'}-\frac{q_i}{q}\varepsilon_{ji'j'}+\frac{1}{1-\nu}\frac{q_iq_j}{q^2}C_{i'j'}\right)$$
$$\times\left(\delta_{il'}C_{jk'}-\frac{q_i}{q}\varepsilon_{jk'l'}+\frac{1}{1-\nu}\frac{q_iq_j}{q^2}C_{k'l'}\right)$$
$$\times D\{Q_{i'k'}\delta_{j'l'}-R(q)[Q_{i'k'}Q_{j'l'}$$
$$+C_{k'j'}C_{i'l'}+S(q)C_{i'j'}C_{k'l'}]\}, \quad \text{(B3)}$$

where the constant D is defined in Eq. (48). Multiplying the expressions in the first two brackets and evaluating the trace over the indices i and j [here and in the following we use the group multiplication properties of the matrices **C** and **Q**, Eq. (53)] yields

$$\delta_{j'l'}Q_{i'k'}-\frac{q_{l'}}{q}\varepsilon_{ji'j'}C_{jk'}-\frac{q_{j'}}{q}\varepsilon_{jk'l'}C_{ji'}$$
$$+\delta_{i'k'}\delta_{j'l'}-\delta_{i'l'}\delta_{j'k'}-\frac{1-2\nu}{(1-\nu)^2}C_{i'j'}C_{k'l'}. \tag{B4}$$

Multiplying this expression by the expression in the square brackets in Eq. (B3) and tracing over the remaining indices we obtain

$$\frac{\Xi_{ij\,ij}(\mathbf{q})}{D}=6-2\frac{1-2\nu}{(1-\nu)^2}-R(q)\left\{10-4\frac{1-2\nu}{(1-\nu)^2}+S(q)\left[6-4\frac{1-2\nu}{(1-\nu)^2}\right]\right\}. \tag{B5}$$

Repeating the same steps, we calculate $\Xi_{ij\,ji}(\mathbf{q})$

$$\frac{\Xi_{ij\ \ ji}(\mathbf{q})}{D}=4-2\frac{1-2\nu}{(1-\nu)^2}-R(q)\left\{10-4\frac{1-2\nu}{(1-\nu)^2}+S(q)\left[6-4\frac{1-2\nu}{(1-\nu)^2}\right]\right\}. \tag{B6}$$

Note that since the above expressions do not depend on the direction of the wave vector **q**, the limit $q\to 0$ can be taken by substituting the corresponding limiting values of R and S instead of functions $R(q)$ and $S(q)$

$$J=\frac{1}{2}\lim_{q\to 0}[\Xi_{ij\,ij}(\mathbf{q})+\Xi_{ij\ \ ji}(\mathbf{q})]$$
$$=D\left[5-2\frac{1-2\nu}{(1-\nu)^2}\right](1-2R)-2DRS\left[3-2\frac{1-2\nu}{(1-\nu)^2}\right]. \tag{B7}$$

The calculation of I proceeds in a similar fashion. After some algebra we obtain

$$I=\lim_{q\to 0}\ \Xi_{ii\,jj}(\mathbf{q})=D\frac{(1-2\nu)^2}{(1-\nu)^2}[2(1-2R)-4RS]. \tag{B8}$$

Substituting the expressions for I and J into Eq. (B2) yields

$$A_i=\frac{D}{1+2\mu D/T}\left[\alpha_i(\nu)-\frac{2\nu\beta_i(\nu)\mu D/T}{1-\nu+2(1+\nu)\mu D/T}\right], \tag{B9}$$

where

$$\alpha_1(\nu)=\frac{1}{2}-\frac{2}{15}\,\frac{(1-2\nu)(2-\nu)}{(1-\nu)^2},$$

$$\alpha_2(\nu)=\frac{1}{3}-\frac{2}{15}\,\frac{(1-2\nu)(3-4\nu)}{(1-\nu)^2}, \tag{B10}$$

$$\beta_1(\nu)=\frac{3}{5}-\frac{4}{15}\,\frac{(1-2\nu)(2-\nu)}{(1-\nu)^2},$$

$$\beta_2(\nu)=\frac{2}{5}-\frac{4}{15}\,\frac{(1-2\nu)(3-4\nu)}{(1-\nu)^2}.$$

APPENDIX C: RADII OF GYRATION OF INTERACTING DISLOCATION LOOPS

The ith $(i=x,y,z)$ component of the radius of gyration of a dislocation loop is defined by

$$R_{gi}^2=\left\langle\left[x_i(0)-\frac{1}{N}\int_0^N x_i(s)ds\right]^2\right\rangle. \tag{C1}$$

To calculate it we use the following chain of equalities

$$x_i(0)-\frac{1}{N}\int_0^N x_i(s)ds=\frac{1}{N}\int_0^N[x_i(0)-x_i(s)]ds$$
$$=-\frac{1}{N}\int_0^N ds\int_0^s ds'\frac{\partial x_i(s)}{\partial s'}$$
$$=-\int_0^N ds\left(1-\frac{s}{N}\right)\frac{\partial x_i(s)}{\partial s'}, \tag{C2}$$

where the last equality follows from Eq. (A7). Substituting Eq. (C2) into Eq. (C1) we find

$$R_{gi}^2=-\frac{\partial^2\ln G_{N0}^B[\mathbf{A}]}{\partial B_i^2}\Bigg|_{\mathbf{B}=0},\qquad G_{N0}^B[\mathbf{A}]\equiv\int d^3x G_{N0}^B[\mathbf{x},\mathbf{x}|\mathbf{A}], \tag{C3}$$

where the vector $\mathbf{B}(s)$ has components $B_i(s)=B_i(1-s/N)$ and the partition function

$$G_{ss'}^B[\mathbf{x},\mathbf{x}'|\mathbf{A}]=\int_{\mathbf{x}(s')=\mathbf{x}'}^{\mathbf{x}(s)=\mathbf{x}}D\mathbf{x}\exp\left\{-\int_{s'}^{s}d\sigma\left[\frac{\partial\mathbf{x}(\sigma)}{\partial\sigma}\right]^2+i\int_{s'}^{s}d\sigma\frac{\partial\mathbf{x}(\sigma)}{\partial\sigma}\cdot[\mathbf{B}(\sigma)+\mathbf{A}(\mathbf{x}(\sigma))\cdot\mathbf{b}]\right\} \tag{C4}$$

obeys the differential equation

$$\left\{\frac{\partial}{\partial s}-\ln z-\frac{a^2}{2}[\nabla-i\mathbf{B}(s)-i\mathbf{A}\cdot\mathbf{b}]^2\right\}G_{ss'}^B[\mathbf{x},\mathbf{x}'|\mathbf{A}]=0 \tag{C5}$$

for $s>s'$ with the initial condition

$$\lim_{s\to s'}G_{ss'}^B[\mathbf{x},\mathbf{x}'|\mathbf{B}]=\delta(\mathbf{x}-\mathbf{x}'). \tag{C6}$$

Note that since the vector $\mathbf{B}(s)$ depends explicitly on s, $G_{ss'}^B$ is a function of both s and s' (and not only of the difference $s-s'$).

Equation (C5) can be rewritten in a gauge-invariant form by introducing the function $\hat{G}^B_{ss'}$:

$$G^B_{ss'}[\mathbf{x},\mathbf{x}'|\mathbf{A}] = \hat{G}^B_{ss'}[\mathbf{x},\mathbf{x}'|\hat{\mathbf{A}}]\exp[i\phi(\mathbf{x})\cdot\mathbf{b} - i\phi(\mathbf{x}')\cdot\mathbf{b}] \tag{C7}$$

with $\nabla^2\phi(\mathbf{x}) = \nabla\cdot\mathbf{A}(\mathbf{x})$. The function $\hat{G}^B_{ss'}[\mathbf{x},\mathbf{x}'|\hat{\mathbf{A}}]$ obeys Eq. (C5) with the substitution $\mathbf{A}\rightarrow\hat{\mathbf{A}} = \mathbf{A} - \nabla\cdot\phi$.

We are looking for the solution of this equation for $\mathbf{A}=0$ in the form

$$G^B_{ss'}(\mathbf{x}) = G^0_{s-s'}(\mathbf{x})\exp[i\mathbf{B}\cdot\mathbf{x}\alpha(s,s') - \mathbf{B}^2a^2\beta(s,s')/2], \tag{C8}$$

where the partition function $G^0_N(\mathbf{x})$ is defined in Eq. (A4). Substituting Eq. (C8) into Eq. (C5) we get the following differential equations for functions $\alpha(s,s')$ and $\beta(s,s')$

$$s\partial\alpha(s,s')/\partial s + \alpha(s,s') - 1 + s/N = 0,$$

$$\partial\beta(s,s')/\partial s = [\alpha(s,s') - 1 + s/N]^2 \tag{C9}$$

with boundary conditions

$$\lim_{s\to s'}\alpha(s,s') = 1 - s'/N, \qquad \lim_{s\to s'}\beta(s,s') = 0. \tag{C10}$$

The solution is

$$\alpha(s,s') = 1 - \frac{s}{2N} - \frac{(s')^2}{2sN},$$
$$\beta(s,s') = \frac{1}{12}\frac{(s+3s')(s-s')^3}{N^2s}. \tag{C11}$$

Substituting Eqs. (C8) and (C11) into (C3) we reproduce the well-known expression for the gyration radius of the Gaussian chain

$$R^2_{gi} = \frac{1}{12}a^2N. \tag{C12}$$

In the case of interacting loops, Eq. (C3) for the radius of gyration is generalized by

$$R^2_{gi} = \frac{1}{T}\frac{\partial^2 F}{\partial B_i^2}\bigg|_{\mathbf{B}=0}, \tag{C13}$$

where the field $\mathbf{B}(s)$ acts on a ''test'' loop of length N and Burgers vector $\mathbf{b}$. We now have to find the partition function of the test loop in the given fields $\mathbf{B}(s)$ and $\mathbf{A}$. Recasting Eq. (A2) into the integrodifferential form we get

$$\hat{G}^B_{N0\mathbf{b}}[\mathbf{x},\mathbf{x}'|\hat{\mathbf{A}}] = G^B_{N0}(\mathbf{x}-\mathbf{x}') - \frac{a^2}{2}\int_0^N dN'\int d^3y\, G^B_{NN'}(\mathbf{x}-\mathbf{y})$$
$$\times\{2i\hat{A}_{ij}(\mathbf{y})b_j\nabla_i + i[\nabla_i\hat{A}_{ij}(\mathbf{y})]b_j$$
$$+\hat{A}_{ij}(\mathbf{y})\hat{A}_{ik}(\mathbf{y})b_jb_k$$
$$+2B_i(N')\hat{A}_{ik}(\mathbf{y})b_k\}\hat{G}^B_{N'0\mathbf{b}}[\mathbf{y},\mathbf{x}'|\hat{\mathbf{A}}]. \tag{C14}$$

Assuming that the field $\hat{\mathbf{A}}$ varies on scales small with respect to the radius of gyration R_g of the loop, we can substitute the unperturbed function $G^B_{N'0}$ in the rhs of Eq. (C14) and get

$$\hat{G}^B_{N0\mathbf{b}}[\hat{\mathbf{A}}] = G^B_{N0}(0)V - \frac{a^2I_N(\mathbf{B})}{2}\int\frac{d^3q}{(2\pi)^3}$$
$$\times\tilde{A}_{ij}(\mathbf{q})\tilde{A}_{kl}(-\mathbf{q})Q_{ik}b_jb_l,$$

$$I_N(\mathbf{B}) = \int_0^N dN'\int d^3x\, G^B_{NN'}(\mathbf{x})G^B_{N'0}(-\mathbf{x}). \tag{C15}$$

Calculating the integrals $I_N(\mathbf{B})$ we find

$$I_N(\mathbf{B}) = \frac{1}{(2\pi a^2N)^{3/2}}\int_0^N dN'$$
$$\times\exp\left\{-\frac{\mathbf{B}^2a^2}{2}[N'(N-N')/N(\alpha(N,N')\right.$$
$$\left.-\alpha(N',0))^2 + \beta(N,N') + \beta(N',0)]\right\}. \tag{C16}$$

We assume that the external field $\mathbf{B}$ can not affect the bare core energy E_b^{bare} per lattice bond and conclude that the free energy F is defined by expression (70) with the renormalized parameter

$$D^R(q_0) = \frac{a^2}{3V}\left[\sum_{N'\mathbf{b}'}n(N',b')N'(b')^2 + I_N(\mathbf{B})b^2\right]. \tag{C17}$$

Taking the derivatives in Eq. (C13) we find

$$R^2_{gi} = \frac{1}{12}a^2N\left\{1 - \frac{17}{35}C_\nu\frac{\mu a^2b^2N}{3\pi T}\left[2\frac{\mu}{T}D^R(q_0)\right]^{1/2}\right\}. \tag{C18}$$

The numerical coefficient in front of the above correction to the Gaussian chain result nearly coincides (within few percent) with that given by the variational procedure (expanded to lowest order in the perturbation). This suggests that the variational procedure gives a reasonable estimate of the size of large loops even when the perturbation result (C18) is no longer valid.

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