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We obtain quantitatively the interaction free energy between two fluctuating dislocation lines that are in contact with a thermal bath. By examining both in-plane and transverse-fluctuation polarizations, we identify attractive and repulsive contributions to the free energy and interpret the results in terms of effective multipolar interactions and the screening of separated lines. We find that the usual form of the dislocation force should be modified to include an additional net attractive force when entropic effects are taken into account.

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I. INTRODUCTION

Interactions among crystalline defects that are mediated by an elastically deformable matrix are central to several important materials phenomena including the formation of Cottrell atmospheres around edge dislocations,1 the development of dislocation microstructures,2 and strain ageing3 along with its dynamic counterpart at elevated temperature, the Portevin-LeChatelier4 effect. Most theoretical treatments of these interactions are, by necessity, couched in terms of idealized elastic models wherein, for example, point defects are regarded as spherical or ellipsoidal centers of dilatation,5,6 line defects (e.g., dislocations) are assumed to be straight or else form simple, closed-loop geometries,6,7 and low-angle grain boundaries are constructed from arrays of dislocations.8 At finite temperature, however, a somewhat more complex picture of defect geometry is required, especially for line and planar defects, in order to account properly for distortions (e.g., kinks and jogs) of entropic origin.

The distortion of dislocation lines can be characterized somewhat more generally in terms of the geometry of topological defects associated with some order parameter. From this unifying perspective, it is possible to formulate analogous descriptions of superconducting flux lines,9 vortex lines in liquid He, and magnetic defects.10 Halsey and Toor,11 for example, have studied fluctuation-induced couplings between dipolar chains in electrorheological fluids and between flux lines in type-II superconductors. They found that thermal fluctuations give rise to forces that, in some cases, dominate over the usual zero-temperature interactions.

With this background in mind, we determine here the low-temperature entropic contributions to the elastic interaction between two dislocations lines that are embedded in an infinite, isotropic elastic continuum. While our approach is similar in some respects to that employed by Halsey and Toor in a related context,11 the present reciprocal-space formulation employs a Green tensor that is appropriate for connecting general dislocation densities. For simplicity, we first consider two screw dislocations that are in equilibrium with a thermal bath, and calculate the interaction energy and associated Helmholtz free energy for this system as a function of defect separation. A multipolar expansion of the dislocation density is then used to classify individual contributions to the interaction energy arising from both in-plane and transverse-fluctuation polarizations. Finally, we characterize the nature of the entropic interaction, extend the treatment to the case of mixed dislocations, and discuss the implications of our results.

II. DISLOCATION-DENSITY TENSOR

A. Straight-screw dislocations

Consider first two straight-screw dislocations embedded in an infinite, isotropic elastic medium, each with line directions along the x3 axis and having Burgers vectors b(1,2) that are displaced by a distance a in the x direction. The relevant components of the dislocation density tensor for these dislocations are

\[ \rho^{(1)}_{ij}(r) = b^{(1)} \delta_{i3} \delta_{j3} \delta(x_1) \delta(x_2), \]

\[ \rho^{(2)}_{ij}(r) = b^{(2)} \delta_{i3} \delta_{j3} \delta(x_1 - a) \delta(x_2) \Theta \left( \frac{L}{2} - x_3 \right) \Theta \left( x_3 + \frac{L}{2} \right), \]

where the first dislocation is evidently infinite in extent while the second dislocation is taken to have a length L. In the subsequent development it will be convenient to work with the corresponding Fourier transforms of these densities,

\[ \rho^{(1)}_{ij}(q) = 2 \pi b^{(1)} \delta_{i3} \delta_{j3} \Theta \left( q_3 \right), \]

\[ \rho^{(2)}_{ij}(q) = b^{(2)} \delta_{i3} \delta_{j3} \exp(iq_1a) \left( \frac{2}{q_3} \right) \sin \left( \frac{q_3 L}{2} \right). \]

The elastic interaction between these straight lines is mediated by a Green function \( G(q) = \mu/q^2 \) (see below), and so the interaction energy per unit length, \( e(a) \), for this pair is then given by

\[ e(a) = \frac{1}{2} m b^{(1)} b^{(2)} \int \frac{d^3 q}{(2 \pi)^3} \frac{1}{q^2} \Theta(q_3) \delta(q_3) \times \left( \frac{2}{q_3 L} \right) \sin \left( \frac{q_3 L}{2} \right) \exp(-q_1a), \]

where \( \mu \) is the shear modulus. Now, since
and the associated force per unit length is given by

\[ F_\kappa(x_3) = \sum_{\kappa=1}^{n_{\text{max}}} \left( c_{+,n,\kappa} e^{in_\kappa \pi x_3 / L} + c_{-,n,\kappa} e^{-in_\kappa \pi x_3 / L} \right), \]

where \( \kappa \) is either \( \perp \) or \( \parallel \), \( L \) is a maximal length characterizing the system, and \( n_{\text{max}} \) is related to a minimum characteristic length. We introduce the wave number \( k_\kappa = 2\pi n_\kappa L / L \) and for convenience write each term in the Fourier expansion as

\[ f_\kappa(x_3) = \Delta_\perp \exp(ik_\parallel x_3) + \Delta_\perp \exp(-ik_\parallel x_3), \]

\[ f_\parallel(x_3) = \Delta_\perp \exp(ik_\parallel x_3) + \Delta_\perp \exp(-ik_\parallel x_3), \]

where \( \Delta_\perp \) (\( \perp \) or \( \parallel \)) are the amplitudes associated with harmonic distortions with wave numbers \( k_\perp(>0) \), respectively, such that \( \Delta_\perp = \Delta_\parallel^* \). The latter condition guarantees that \( f_\parallel(x_3) \) is real and the restriction to nonzero wave numbers implies that the line is, on average, along the \( x_3 \) axis.

The dislocation density for this case can be obtained by first constructing a unit tangent \( \mathbf{t} \) to the dislocation line. For the given profile

\[ \mathbf{t} = \frac{x_3 + \dot{x}_3 \mathbf{\partial f}_3(x_3)}{1 + \left( \mathbf{\partial f}_3(x_3) \right)^2} \]

Next, upon integrating dislocation “point” sources along the arc length \( s \) of the perturbed line one obtains

\[ \rho_{ij}^{(1)}(r) = \delta_{j3} \int_{-\infty}^{\infty} ds \delta(x_1 - f_i(x_3')) \delta(x_2 - f_\parallel(x_3')) \times \delta(x_3 - x_3') \mathbf{t}_i(x_3') \]

\[ = \delta_{j3} \left[ \delta_{13} \frac{\partial f_1(x_3)}{\partial x_3} + \delta_{23} \frac{\partial f_2(x_3)}{\partial x_3} \right] \times \delta(x_1 - f_i(x_3)) \delta(x_2 - f_\parallel(x_3)), \]

where \( ds = \sqrt{(dx_1)^2 + (dx_2)^2 + (dx_3)^2} \). A similar expression can be written for dislocation 2, except that the perturbation profile wave number will be \( k_\perp \) and that, as above, we restrict the line at this stage to the interval \((-L/2, L/2)\). Finally, it should be noted that the dislocation densities defined above are solenoidal (i.e., \( \partial_i \rho_{ij} = 0 \)) in the limit \( L \to \infty \), as required by topological constraints.

It is again convenient to work with the Fourier-transformed densities. While it is possible to write these densities in terms of infinite-series expansions, it is more useful here to restrict attention to the lowest-order terms in the amplitudes \( \Delta_\perp \). Physically, this amounts to focusing on those small-amplitude line fluctuations induced at relatively low temperatures. In short, to second-order in the fluctuation amplitudes, one finds for dislocation 1 that

FIG. 1. A schematic showing two fluctuating dislocation lines, each with its Burgers vector along \( x_3 \), that are separated by a distance \( a \) along the \( x_1 \) direction. For clarity, only one possible fluctuation polarization is shown here. \( \lambda \) denotes wavelength here.

\[ \int d^2q \frac{1}{q^2} \exp(-iq_1a) = -2\pi \ln(a), \]

one finds that

\[ e(a) = e_{\text{straight}}(a) = -\frac{\mu b^{(1)} b^{(2)}}{2\pi} \ln(a), \]

and the associated force per unit length is given by

\[ \frac{d}{da} e(a) = \frac{\mu b^{(1)} b^{(2)}}{2\pi a}. \]

Thus, the interaction between screw dislocations having the same (opposite) Burgers vectors is repulsive (attractive) in nature.

B. Perturbed dislocation lines

Now suppose that harmonic perturbations are added to the aforementioned straight-screw dislocation lines without changing the Burgers vector, which remains along the \( x_3 \) axis. This is shown schematically in Fig. 1 for one possible fluctuation polarization. Such perturbations might arise from thermal fluctuations in the medium. For example, isolated jogs can be regarded as short steps that displace the dislocation line from one slip plane to another, and individual kinks are short elements that displace the line within a given slip plane.\cite{12,13} Consequently, an idealized jog that nucleates on an initially straight-screw dislocation is associated with local climb, endowing the dislocation with edge character. A general distortion, then, can be viewed as a superposition of modes having screw, edge, and mixed character that is amenable to Fourier analysis. This is perhaps most easily accomplished by parametrizing the line position in the \( x_1-x_2 \) plane as \( \mathbf{r} = \hat{x}_1 F_1(x_3) + \hat{x}_2 F_\parallel(x_3) \) where

\[ F_\kappa(x_3) = \sum_{\kappa=1}^{n_{\text{max}}} \left( c_{+,n,\kappa} e^{in_\kappa \pi x_3 / L} + c_{-,n,\kappa} e^{-in_\kappa \pi x_3 / L} \right), \]
\[ \frac{\rho_{ij}^{(1)}(q)}{2\pi b^{(1)}} = \delta_{ij} \delta_{j3} \left[ \delta(q_3) + i q_2 F_{+1}(k_\perp) - \frac{q_2^2}{2} G_{+1}(k_\perp) \right. \\
+ i q_1 F_{+1}(k_\perp) - \frac{q_1^2}{2} G_{+1}(k_\perp) + \cdots \left. \right] \\
+ i \{ \delta_{ij} \delta_{j3} k_1 \left[ F_{+1}(k_\perp) + i q_2 G_{+1}(k_\perp) \right] + \delta_{ij} \delta_{j3} k_1 \left[ F_{-1}(k_\perp) + i q_1 G_{-1}(k_\perp) \right] + \cdots \} \quad (11) \]

where

\[ F_\pm(k) = \Delta_\pm \delta(q_3 + k) \mp \Delta_\pm \delta(q_3 - k), \]

\[ G_\pm(k) = \Delta_\pm^2 \delta(q_3 + 2k) \pm \Delta_\pm \delta(q_3 - 2k) \\
+ (\Delta_\pm \Delta_\perp \mp \Delta_\perp \Delta_\pm) \delta(q_3) \quad (12) \]

for both the parallel (\( \parallel \)) and perpendicular (\( \perp \)) components. The corresponding tensor density for dislocation 2 can be obtained from Eq. (11) upon incorporating a factor of \( \exp(-iq_1a) \) to reflect the separation of the lines and making the substitutions

\[ b^{(1)} \rightarrow b^{(2)}, \]

\[ k_{1\perp} \rightarrow k_{1\perp}', \]

\[ 2\pi \delta(q_3 \pm k_{1\perp}') \rightarrow D(q_3 \pm k_{1\perp}') = \frac{2 \sin \left( \frac{q_3 \pm k_{1\perp}'}{L} \right)}{q_3 \pm k_{1\perp}'} \quad (13) \]

### III. ENERGETICS

Having determined the dislocation-density tensor, the aim here is to calculate the interaction energy between two perturbed dislocation lines. This energy will, in turn, determine the corresponding Boltzmann weight for the fluctuating pair of lines and, hence, the equilibrium statistical mechanics of this system. For this purpose, we extract first the interaction term from an expression for the total energy \( E \) derived by Kosevich and reexpressed by Nelson and Toner as an integral over reciprocal space given by

\[ E = \frac{1}{2} \int \frac{d^3 q}{(2\pi)^3} K_{ijkl}(q) \rho_{ij}(q) \rho_{kl}(-q). \quad (14) \]

where the kernel (without core energy contributions)

\[ K_{ijkl} = \frac{\mu}{q} \left[ Q_{ij} Q_{kl} + C_{ij} C_{kl} + \frac{2\nu}{1-\nu} C_{ij} C_{kl} \right]. \quad (15) \]

In Eq. (15), the projection operators \( Q_{ij} \) and \( C_{ij} \) are defined as

\[ Q_{ij} = \delta_{ij} - \frac{q_i q_j}{q^2}, \]

\[ C_{ij} = \epsilon_{ijk} \frac{q_k}{q}, \quad (16) \]

and \( \epsilon_{ijk} \) are the components of the Levi-Civita tensor density. We note that the energetics of the disordered core regions near each line can be incorporated, at least approximately, by the inclusion of a phenomenological energy-penalty term in the kernel above. Further, because the dislocation-density tensor is solenoidal, we can rewrite the above kernel in a more convenient form as

\[ K'_{ijkl} = \frac{\mu}{q} \left[ \delta_{ij} Q_{jl} + C_{ij} C_{kj} + \frac{2\nu}{1-\nu} C_{ij} C_{kl} \right]. \quad (17) \]

It is this last kernel that will be employed in the development below, and therefore, to simplify the notation, the prime will be omitted.

Upon inserting Eq. (11) and the corresponding density for dislocation 2 into Eq. (14) and restricting attention to the interaction-energy terms, one can calculate the net interaction energy per unit length, \( e(a) \). As the densities are given to second order in the fluctuation amplitudes, we will determine the interaction energy to the same order in \( \Delta_\perp \). For both bookkeeping and interpretive purposes it is convenient to classify the contributions to \( e(a) \) in terms of the character of the interactions (i.e., screw-screw, edge-screw, and edge-edge) and their order in the fluctuation amplitudes.

We note that one can do the analysis in an equivalent fashion using a direct representation of the dislocation-density tensor. This approach is outlined in Appendix A and yields, as it should, exactly the same expressions as those presented next.

### Contributions to the interaction energy

We begin by considering interactions between segments having different character. The edge-screw interactions are mediated by \( K_{1333} = K_{3333} \). As is evident from Eq. (17), both of these kernels vanish. Thus, edge and screw segments on the different perturbed lines do not interact. This result can also be seen from equivalent line-integral expressions for the interaction energy between dislocation loops.\(^{1,14}\)

For the case of screw-screw interactions, the zeroth-order contribution to the energy is the same as that for two straight, infinite dislocations [see Eq. (5)]. More generally, the interaction of the screw segments is mediated by \( K_{3333}(q) \). It then follows that the first-order contributions to the interaction energy vanish while the second-order contributions are non-vanishing and are given by

\[ \frac{\mu}{(2\pi)^3} b^{(1)} b^{(2)} \left[ A(\parallel) S_1(k_\parallel, a) + A(\perp) S_2(k_\perp, a) - B(\parallel) T_1(a) \right. \]

\[ - B(\perp) T_2(a) \left. \right], \quad (18) \]

where the amplitude functions are given by
where the nonzero contributions to the interaction energy are frequently, in-plane and transverse-edge segments do not couple fluctuations to second order in \( D \) and, consequently, the self-energy of the system, we find that the remaining functions are defined by

\[
A(||) = \left[ \Delta_{+1||}^{(1)} \Delta_{-1||}^{(2)} + \Delta_{+1||}^{(2)} \Delta_{-1||}^{(1)} \right] \delta_{k_1, k_2}^{(1)},
\]

\[
B(||) = \left[ \Delta_{+1||}^{(1)} \Delta_{-1||}^{(2)} + \Delta_{+1||}^{(2)} \Delta_{-1||}^{(1)} \right].
\] (19)

Note that the Kronecker delta in Eq. (19) (for terms involving \( n \)) the values of \( n \) in the Fourier sums given in Eq. (7) to be the same for both lines. The integrals \( S_i \) and \( T_i \) (\( i = 1, 2 \)) appearing in Eq. (18), along with other integrals needed below, are evaluated in Appendix B. Upon considering the amplitude expansion that led to Eq. (18), it is evident that the terms involving \( S_i \) arise from dipolar interactions between lines, while those involving \( T_i \) link line-monopole and quadrupolar interactions.

Finally, the edge-edge interactions are mediated by \( K_{1323} \) and \( K_{1313} \). It can be shown that the kernels \( K_{1323} = K_{1313} \) do not connect fluctuations to second order in \( \Delta \) and, consequently, in-plane and transverse-edge segments do not couple here. The nonzero contributions to the interaction energy are then

\[
\frac{\mu}{(2\pi)^2} b^{(1)} b^{(2)} \left[ A(||) k_1^2 \right. \left. V(k_1, a) + \left( \frac{1}{1 - \nu} \right) W_2(k_1, a) \right] + A(\perp) k_2^2 \left[ V(k_2, a) + \left( \frac{1}{1 - \nu} \right) W_1(k_2, a) \right].
\] (20)

where, again, the integrals \( V \) and \( W_i \) (\( i = 1, 2 \)) are tabulated in Appendix B. The fact that the integrals \( S_i \) involve modified Bessel functions implies that line fluctuations effectively screen the "bare" screw dislocation with a screening length that is proportional to the fluctuation wavelength. Moreover, as in the case of screw-screw interactions, edge-edge interactions also couple line multipoles having net even order (at least to second-order in the fluctuation amplitudes).

Upon combining the various contributions to the energy with the self-energy of the system, we find that

\[
e(a) = e_{\text{self}} + e_{\text{straight}} + \frac{\mu b^{(1)} b^{(2)}}{(2\pi)^2} \left[ \alpha_i(k_1, a) A(||) + \alpha_1(k_2, a) A(\perp) - T_1(a) B(||) - T_2(a) B(\perp) \right],
\] (21)

where

\[
e_{\text{self}} = \sum_{i=1}^{2} \frac{\mu}{4\pi} \left( \frac{b^{(i)}}{b^{(j)}} \right)^2 \ln \left( \frac{L}{b^{(j)}} \right) \left[ 1 + \left( \frac{1 + \nu}{1 - \nu} \right) \left( k^{(i)} \right)^2 \Delta_{+1||}^{(i)} \Delta_{-1||}^{(j)} \right] + \left( k^{(i)} \right)^2 \Delta_{+1||}^{(i)} \Delta_{-1||}^{(j)}
\] (22)

and, in order to simplify the notation, \( k^{(i)} = k, k^{(2)} = k' \). The remaining functions are defined by

\[
\alpha_i(k_1, a) = S_i(k_1, a) + k_1^2 \left[ V(k_1, a) + \left( \frac{1}{1 + \nu} \right) W_2(k_1, a) \right],
\]

\[
\alpha_1(k_2, a) = S_2(k_2, a) + k_2^2 \left[ V(k_2, a) + \left( \frac{1}{1 - \nu} \right) W_1(k_2, a) \right].
\] (23)

IV. HELMHOLTZ FREE ENERGY

The Helmholtz free energy and, therefore, the associated finite-temperature forces can be obtained by first constructing the partition function \( Z(k, k') \) for the system corresponding to a vector \( k = \hat{k}_x + j_k \) and \( k' = \hat{k}_x + j_k' \). This is accomplished by considering the change in energy, \( \Delta e(a) \), associated with fluctuations on two initially straight-screw dislocations and noting that it can be written as a sum of contributions, \( \Delta e \) and \( \Delta e \), corresponding to in-plane and transverse-fluctuation modes. Thus, the factorized partition function

\[
Z(k, k') = N \left( \int d\omega \exp \left( \frac{-L(\Delta e)}{k_B T} \right) \right) \times \left( \int d\omega \exp \left( \frac{-L(\Delta e)}{k_B T} \right) \right),
\] (24)

where \( N \) is a normalization factor and \( \omega \) is the eight-dimensional configuration space described by the complex fluctuation amplitudes.

The total change in energy relative to two straight-screw dislocations is the sum of the expression in Eq. (21) (less contributions from \( e_{\text{straight}} \) and the self-energy of the straight lines) over \( n_{||} \) and \( n_{\perp} \) on the two dislocation lines (recognizing that \( k_x = 2n_x \pi / L \), where \( \kappa \) is either \( \perp \) or \( || \)). Putting those sums in the exponential in Eq. (24), we see that each contribution to \( Z \) in Eq. (24) is a Gaussian integral. Integrating over all amplitudes [remembering the Kronecker delta in Eq. (19)], we find that the perpendicular contribution to the partition function is given, subject to certain restrictions, by

\[
\ln(Z_{||}) = \sum_{n_{||}=n_{\text{min}}}^{n_{||}=n_{\text{max}}} \ln \left( \frac{8\pi^3 k_B T}{L \mu b^{(1)} b^{(2)} \left[ d^{(1)}(k) - T_2 \right]} \right) + \sum_{n_{\perp}=n_{\text{min}}}^{n_{\perp}=n_{\text{max}}} \ln \left( \frac{8\pi^3 k_B T}{L \mu b^{(1)} b^{(2)} \left[ d^{(2)}(k) - T_2 \right]} \right) - \sum_{n_{\perp}=n_{\text{min}}}^{n_{\perp}=n_{\text{max}}} \ln \left( 1 - \left[ d^{(1)}(k) - T_2 \right] \left[ d^{(2)}(k) - T_2 \right] \right),
\] (25)

where

\[
d^{(i)}(k) = \frac{\pi b^{(i)}}{b^{(j)}} \ln \left( \frac{L}{b^{(j)}} \right) \left( \frac{1 + \nu}{1 - \nu} \right) k^2 \quad (j \neq i),
\] (26)

\( \kappa \) is either \( || \) or \( \perp \), and the term coming from the normalization has, for convenience, been ignored. The \( || \) contribution is
similar in form to Eq. (25), substituting $T_1$ for $T_2$ and all $\perp \rightarrow \parallel$. Note that in the quantities in the sums in Eq. (25), all $k = 2n\pi/L$.

To evaluate the sums in Eq. (25), we recognize that the characteristic length $L$ is large enough that we can take $k_\alpha = 2n\pi/L$ as a continuous variable and integrate, where

$$k_{\min} = 2\pi/L, \quad k_{\max} = 2\pi\lambda, \quad \text{and} \quad \lambda \text{ is some characteristic length that characterizes the smallest fluctuation in the system, i.e., some small number of Burgers vectors.}$$

The aforementioned restriction, implicit in Eq. (25), is that the matrix $\tilde{M}$ associated with the quadratic form for $\Delta \epsilon(a)$ be positive definite or, equivalently, have positive eigenvalues. Upon analyzing the spectrum of $\tilde{M}$, it is evident that a meaningful partition function can be obtained for sufficiently large separations $a > a_{\text{crit}}$, where $a_{\text{crit}}$ is the value for a critical separation, such that the self-energy change resulting from line deformation offsets the attractive, transverse monopole-quadrupole line interaction. In practice, $a_{\text{crit}}$ is the zero of the function $\{[d^{(i)}_1(k_{\min}) - a][d^{(i)}_2(k_{\min}) - a]\} - \alpha_i^2$.

The parallel contribution to the partition function is given by

$$\ln(Z_{\parallel}) = \ln(Z_{1(\parallel)}) + \ln(Z_{2(\parallel)}) + \ln(\Delta Z_{\parallel}), \quad \text{(28)}$$

where

$$\ln(Z_{1(\parallel)}) = \frac{L}{2\pi} \left[ k_{\max} \ln \left( \frac{8e^2\pi^3 T}{L\mu b^{(1)}b^{(2)}} \right) \left( \frac{1}{d^{(i)}_1(k_{\max}) + 2\pi/a^2} \right) \right]$$

$$- k_{\min} \ln \left( \frac{8e^2\pi^3 T}{L\mu b^{(1)}b^{(2)}} \right) \left( \frac{1}{d^{(i)}_1(k_{\min}) + 2\pi/a^2} \right)$$

$$- \frac{2}{\alpha} \left( \frac{2\pi k^2}{a} \right)^{1/2} \left\{ \tan^{-1}\left[ a\sqrt{d^{(i)}_1(k_{\min})/2\pi} \right] \right\}, \quad \text{(29)}$$

and

$$\ln(\Delta Z_{\parallel}) = - \frac{L}{2\pi} \int_{k_{\min}}^{k_{\max}} \ln \left[ \alpha_i^2 \left( d^{(i)}_1 + 2\pi/a^2 \right)(d^{(i)}_2 + 2\pi/a^2) \right] dk. \quad \text{(30)}$$

The term in Eq. (30) must be evaluated numerically.

The perpendicular component of the partition function is given by

$$\ln(Z_{\perp}) = \ln(Z_{1(\perp)}) + \ln(Z_{2(\perp)}) + \ln(\Delta Z_{\perp}), \quad \text{(31)}$$

where

$$\ln(Z_{1(\perp)}) = \ln(Z_{1(\parallel)}) + \ln(Z_{2(\parallel)}) + \ln(\Delta Z_{\parallel}), \quad \text{(28)}$$

$$\ln(\Delta Z_{\perp}) = - \frac{L}{2\pi} \int_{k_{\min}}^{k_{\max}} \ln \left[ \alpha_i^2 \left( d^{(i)}_1(k_{\min}) - a \right) \left( d^{(i)}_2(k_{\min}) - a \right) \right] dk, \quad \text{(33)}$$

where the final integral must be evaluated numerically.

The Helmholtz free energy associated with the interactions between the fluctuating screws is then given by

$$A = -k_BT \ln(Z_{\parallel}) - k_BT\{\ln(Z_{\parallel}) + \ln(Z_{\perp})\}. \quad \text{(34)}$$

V. TEMPERATURE-DEPENDENT FORCE

The average force (by convention we use $F$) between the dislocations is given by

$$\langle F(a) \rangle = \frac{k_BT}{L} \frac{\partial \ln Z_{\parallel}}{\partial a}$$

$$= \langle F^{(1)}(a) \rangle + \langle F^{(2)}(a) \rangle + \langle F^{(1)}(a) \rangle + \langle F^{(2)}(a) \rangle$$

$$+ \langle \Delta F_{\parallel}(a) \rangle + \langle \Delta F_{\perp}(a) \rangle, \quad \text{(35)}$$

where

$$\langle F^{(i)}(a) \rangle = \frac{k_BT}{L} \frac{\partial \ln Z^{(i)}_{\parallel}}{\partial a}$$

$$= \frac{2k_BT}{\pi} \left( \frac{2\pi k^2}{a} \right)^{1/2} \frac{1}{a} \left\{ \tan^{-1}\left[ a\sqrt{d^{(i)}_1(k_{\min})/2\pi} \right] \right\}$$

$$- \tan^{-1}\left[ a\sqrt{d^{(i)}_1(k_{\min})/2\pi} \right], \quad \text{(36)}$$

$$\langle F^{(i)}(a) \rangle = \frac{k_BT}{L} \frac{\partial \ln Z^{(i)}_{\perp}}{\partial a}$$

$$= \frac{2k_BT}{\pi} \left( \frac{2\pi k^2}{a} \right)^{1/2} \frac{1}{a} \left\{ \tanh^{-1}\left[ a\sqrt{d^{(i)}_1(k_{\min})/2\pi} \right] \right\}$$

$$- \tanh^{-1}\left[ a\sqrt{d^{(i)}_1(k_{\min})/2\pi} \right], \quad \text{(37)}$$

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In Eq. (38), \( \kappa \) is either \( \perp \) or \( \parallel \) and the integral must be evaluated numerically.

**VI. NUMERICAL RESULTS**

To be more explicit, let us consider a system in which the interacting dislocations have the same properties. Further, we will use the material parameters for copper, namely, \( \nu = 0.25, \mu = 54.64 \) GPa, and \( b = 2.56 \) \( \text{Å} \), and take as the maximum length of the system, \( L = 200b \), and a minimum length of \( 10b \). For convenience, we measure the distance between the dislocations in units of \( b \) (i.e., \( a = a^* b \)). For the parameters chosen here, the minimum value of \( a^* \) for which we have an analytic solution is \( a^* = 21.17 \).

Figure 2 shows the average normalized force \( \langle F \rangle/k_B T \) between dislocations versus normalized separation \( a^* \). Also shown are the contributions to that force from \( \Sigma_{\kappa}(\Delta F_{\kappa}(i)) \) and \( \Sigma_{\kappa}(\Delta F_{\kappa}) \). It should be noted that, because of the singularity in \( \langle \Delta F_{\perp} \rangle \), \( a^* \) is restricted to values greater than \( a^*_{\text{crit}} \). From the figure it can be seen that the contributions to the force are attractive and have roughly the same magnitude. At \( a^* = 22 \), the net force due to fluctuations is approximately \( -0.001 k_B T / b^2 \). Using the value of \( b \) given above, we see that at a temperature of \( 600 \) K, the thermal force is approximately \( 1.3 \times 10^{-4} \) J/m\(^2\). The direct force between two straight screws is given by Eq. (6). With the parameters given above, at \( a^* = 22 \) that force is approximately \( 0.10 \) J/m\(^2\) or a factor of about \( 1000 \) greater.

It is of interest to estimate the magnitude of the average force for smaller dislocation separations where it is expected to be substantially larger. While the second-order expansion in fluctuation amplitudes employed here necessarily restricts the range of \( a^* \) that can be explored, a careful examination of the various contributions to the total force is, nevertheless, revealing. The thermal force is a balance between a number of terms, all having roughly the same magnitude. Figure 3 shows the net parallel and perpendicular contributions to this force, indicating that the parallel (perpendicular) contributions are repulsive (attractive), yet similar in magnitude. Despite the singularity in the perpendicular term that sets the minimum dislocation separation at \( a^*_{\text{crit}} \), we can evaluate the parallel contributions to the force at smaller separations and, hence, consider thermally induced interactions for that specific polarization. Indeed, for the parallel contribution to the force, we can take \( k_{\min} \to 0 \) and \( k_{\max} \to \infty \) and find that \( F_\parallel \approx k_B T / a^2 \). The dependence of the average force on \( a \) can be understood in terms of the multipolar character of the line-line interactions averaged over the spectrum of line fluctuations. At \( a^* = 2 \), for example, the thermal contributions are about \( 10\% \) of the direct interactions. Since the thermal contributions fall off as \( 1/a^2 \) and the direct force as \( 1/a \), the thermal contributions are relatively less important at larger separations. Finally, a more complete description of the energetics at small separation can be obtained by extending the formalism outlined above to include interactions to higher order in the fluctuation amplitude, or by a numerical evaluation of Eq. (14) upon substituting the Fourier transform of the densities given by both Eq. (10) and its modification for a dislocation translated by a distance \( a \).
VII. DISCUSSION AND CONCLUSIONS

From an analysis of the energetics of interacting screw dislocations that are in contact with a thermal bath, we have shown that the usual interaction is modified by entropically generated kinks and jogs. The Helmholtz free energy and associated force were calculated for a system containing fluctuating lines, and the various contributions to the interaction were interpreted in terms of the defect character of thermally induced modes. It was shown that thermal defects on a line lead to an effective screening of separated dislocations and, ultimately, to a net attractive force between the lines, which should properly be incorporated in finite-temperature studies of dislocation energetics, at least at small dislocation separations.

It is worth noting that thermally induced line interactions can alter the energetics and dynamics of an ensemble of dislocations and/or systems containing both point and line defects. In the former case, thermal fluctuations may lead to disorder in a Taylor lattice, the analog of an Abrikosov flux lattice\(^9\) for dislocations. The impact of disorder on lattice stability and, therefore, mechanical properties remains an open question. In the latter case, point defects can pin dislocations\(^17\) and pinning effectiveness is determined, at least in part, by kink/jog distributions. Thus, a more complete picture of dislocation mobility at finite temperature centers around the statistical mechanics of line fluctuation-solute interactions.

Although we have focused here on the interaction of screw dislocations, the generalization of our approach to describe edge and/or mixed dislocations is straightforward. For example, the interaction between two edges with line directions along \(x_3\) and Burgers vectors along \(x_1\) is mediated by \(K_{311}\) and so, for straight lines displaced by \(r = \hat{x}_1 a_1 + \hat{x}_2 a_2\), one obtains an interaction energy per unit length,

\[
e(a) = \frac{2\mu b^{1(b/2)}(b/2)}{(2\pi)^2(1-\nu)} \int d^2 q \frac{q_2^2}{(q_1^2 + q_2^2)^{3/2}} \exp\left[-i(q_1 a_1 + q_2 a_2)\right]
\]

\[
e(a) = \frac{\mu b^{1(b/2)}(b/2)}{4(1-\nu)} \left[\ln(a_1^2 + a_2^2) + \frac{2a_2^2}{a_1^2 + a_2^2}\right]. \tag{39}\]

Given this equation, one can now consider the effect of line perturbations on the energetics of interacting dislocations originally having pure edge character. It is expected that this system is also describable in terms of coupled line multipoles with an interaction energy that reflects the screening of the undeformed line by thermal defects.

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APPENDIX A

If the direct form of the dislocation-density tensor\(^21\) is used, the free energy can be written as

\[
E = -\frac{\mu}{8\pi} \int_0^\infty \int_{-\infty}^{\infty} \frac{1}{2} \left[\epsilon_{ij} \epsilon_{jmn} \rho_i(r) \rho_{jm}(r') \right. \\
+ \epsilon_{ij} \epsilon_{mn} \rho_{ij}(r) \rho_n(r') \left. + \frac{\nu}{1-\nu} \epsilon_{ij} \epsilon_{mn} \rho_{ij}(r) \rho_{mn}(r') \right] T_{mp}(r,r') dr dr', \tag{A1}\]

where

\[
T_{mp}(r,r') = \frac{\delta^2[r'-r]}{\partial x_p \partial x_m} = -\delta_{np} \frac{\delta^2[r'-r]}{[r'-r]^3} + \frac{(x_p'-x_p)(x_m'-x_m)}{[r'-r]^3}. \tag{A2}\]

and \(\rho_{ij}\) are components of the dislocation-density tensor. In Eq. (A1), \(\epsilon_{ijk}\) is the Levi-Civita tensor. Since for the problem under consideration here \(\rho_{11}, \rho_{22},\) and \(\rho_{33}\) are the only non-zero components of the dislocation-density tensor, Eq. (A1) simplifies greatly.

Using the dislocation-density tensor given in Eq. (10), we integrate over the \(\delta\) functions and expand to second order in the displacements \(\Delta a_i\). Using the integrals outlined in Appendix B, we arrive at the same energy expressions as given above using the Fourier representation.

APPENDIX B

The integrals needed in Sec. III are tabulated here. The subscript \(i\) takes on the values 1 and 2 and \(K_0(ka)\) and \(K_2(ka)\) are modified Bessel functions of the second kind.\(^{18}\) It should be noted that one convenient method for calculating the integrals is to observe that they are derivable by differentiating the generating integral

\[
I(\alpha) = \int \frac{d^2 q}{q_1^2 + q_2^2 + k^2} \exp(-i\alpha a) = 2\pi K_0(\alpha) \tag{B1}\]

and using recurrence relations for the modified Bessel functions\(^{19,20}\) to express the results in terms of \(K_0(\alpha)\) and \(K_2(\alpha)\). The integrals referred to in the text are

\[
S_i(k,a) = \int d^2 q \frac{q_i^2}{q_1^2 + q_2^2 + k^2} \left(1 - \frac{k^2}{q_1^2 + q_2^2 + k^2}\right) \exp(-i\alpha a) \\
= \pi k^2[K_2(\alpha) - 2K_0(\alpha)]\delta_{i2} - \pi k^2 \left[\frac{2}{2} + \frac{(\alpha k)^2}{2} K_0(\alpha) + \frac{1}{2} (\frac{2}{2} K_2(\alpha) \right] \delta_{i1}, \tag{B2}\]

\(\delta_{ij}\) is the Kronecker delta.
\[ T_i(a) = \int d^2 q \frac{q_i^2}{q_1^2 + q_2^2 + k^2} \exp(-iq_1 a) = \frac{-2\pi}{a} (\delta_{i1} - \delta_{i2}), \]  
(B3)

\[ V(k,a) = \int d^2 q \frac{1}{q_1^2 + q_2^2 + k^2} \left( 1 - \frac{k^2}{q_1^2 + q_2^2 + k^2} \right) \exp(-iq_1 a) \]
\[ = \pi \left[ \frac{(ka)^2}{2} K_0(ka) - \frac{(ka)^2}{2} K_2(ka) \right], \]  
(B4)

\[ K_{\nu}(x) = \frac{\Gamma(\nu + \frac{1}{2})}{2\Gamma(\frac{1}{2})} \left( \frac{2x}{\nu} \right)^{\nu} \int_{-\infty}^{\infty} e^{itx} \frac{e^{itx}}{t^{\nu+1+\nu}} dt. \]  
(B6)

15. The fluctuation amplitudes and, hence, the measure can of course be written in terms of real variables, namely, the real and imaginary parts of the amplitudes.
16. An approximation to the critical separation can be obtained by neglecting line dipolar interactions and assuming that the two dislocations have the same properties and fluctuation wavelengths. In this case, \( a_{crit} \approx \sqrt{2/[\ln(L/b)(1+\nu)(1-\nu)(1/k_{ij})]}. \)