Evolution of the correlation functions in two-dimensional dislocation systems

Péter Dusán Ispánovity,[1,*] István Groma,[1,†] and Géza Györgyi[2,3,‡]

[1]*Department of Materials Physics, Eötvös University, H-1117 Budapest, Pázmány sétány 1/a, Hungary*

[2]*Institute of Theoretical Physics, HAS Research Group, Eötvös University, H-1117 Budapest, Pázmány sétány 1/a, Hungary*

[3]*Research Institute for Solid State Physics and Optics, H-1525 Budapest, P.O. Box 49, Hungary*

(Received 8 May 2008; published 29 July 2008)

In this paper, spatial correlations of parallel edge dislocations are studied. After closing a hierarchy of equations for the many-particle density functions by the Kirkwood superposition approximation, we derive evolution equations for the correlation functions. It is found that these resulting equations and those governing the evolution of density fields of total as well as geometrically necessary dislocations around a single edge dislocation are formally the same. The second case corresponds to the already described phenomenon of Debye screening of an individual dislocation. This equivalence of the correlation functions and screened densities is also demonstrated by discrete dislocation dynamics simulation results, which confirm the physical correctness of the applied Kirkwood superposition approximation. Relation of this finding and the linear-response theory in thermal systems are also discussed.

DOI: 10.1103/PhysRevB.78.024119 PACS number(s): 62.20.F−, 05.90.+m, 61.72.Lk

I. INTRODUCTION

It is well known that plastic deformation of crystalline materials is caused by the motion of a large number of interacting dislocations. Although the properties of individual dislocations have been known for decades, the question of how to build up a micronscale level continuum description of dislocations is still an unresolved issue in the theory of crystal plasticity. The appropriate continuum theory could provide a framework for understanding dislocation pattern formation or size effects.

Several phenomenological models have been proposed for dislocation patterning so far. Here, we first mention the work of Walgraef and Aifantis,[1,2] who adopted a reaction-diffusion model from the description of oscillating chemical reactions. In their model, second-order gradient terms are introduced to account for the spatial fluctuations of the dislocation density. Although the framework turned out to be very successful in the prediction of different dislocation structures, the physical origin of the length scales introduced through the coefficients of the gradient terms is not really understood. The same problem applies to the model of Kratochvíl and co-workers,[3,4] in which nonlocal terms are introduced for describing spatial interactions through the sweeping mechanism.

In a nonphenomenological model proposed by Groma,[5] a system of parallel edge dislocations in single slip was studied. By performing ensemble averaging on statistically equivalent dislocation distributions, a chain of equations for the many-body dislocation density fields was derived. First, dislocation correlations were neglected, which corresponds to a mean-field approximation.[6] Here, the stress acting on dislocations is simply the "self-consistent" field, which is the long-range stress field of the geometrically necessary dislocations. If the dislocation system is correlated, which is indeed the case for real systems (see, e.g., in Ref. 7), further stresslike terms appear in the constitutive equations.[8] The most important nontrivial term is the gradientlike "back stress," which can be interpreted as the short-range effect of dislocation pileups. In order to check the validity of this two-dimensional (2D) theory, its predictions were compared to discrete dislocation dynamics simulation results; good agreement was found.[9,10]

There are several current approaches in the literature to develop a density-based continuum model for three dimensions (3D). El–Azab based his theory on Nye's dislocation density tensor.[11] After studying the mean-field approximation of an uncorrelated ensemble in their recent paper, El–Azab *et al.*[12,13] turned to the investigation of dislocation correlations on simulated 3D dislocation ensembles in a body-centered-cubic crystal. Csikor *et al.*[14] reported about a complementary numerical study, focused on the range of 3D dislocation pair correlations in face-centered-cubic materials. Recently, another promising theory has been proposed by Hochrainer and co-workers,[15–17] who studied the evolution of dislocation lines in a higher-dimensional space. Motivated by the 2D results, dislocation correlations are introduced into the theory semiphenomenologically by considering short-range stress terms, such as the aforementioned back stress.[17] Similar extension was adopted by Schwarz *et al.*[18] too for a continuum theory of interacting curved dislocations.[19] In all mentioned current 3D continuum theories of dislocation dynamics, one of the biggest challenges is the precise incorporation of the effects of dislocation correlations, which seems to be unavoidable. So, the investigation of the evolution of the correlation properties is of great importance, but even in 2D, this problem has not been solved yet.

In the past two years, light has been shed on equilibrated dislocation systems by the discovery of the effect of dislocation screening.[20,21] Its most direct physical significance is that it explains the extensivity of the elastic energy in equilibrium by the appropriate relative arrangement of the dislocations, resulting generically in a finite interaction length, rather than the unscreened infinite range interaction. On the technical side, in the simplest example represented by a 2D single slip, edge dislocation system, an effective thermodynamic potential was proposed for the purpose of the variational calculation of the geometrically necessary density. Summarizing the results for large and constant total dislocation density, and for small but variable geometrically necessary density, the equation for the induced density with arbitrary external dislocations was constructed and its Green's function for infinite boundary conditions was given analytically. Hence, the induced density and the resulting screened elastic potential by a single external dislocation was obtained, showing suppression in all directions exponentially strong except for one axis, where it was of power type. This phenomenon bears close resemblance to Debye screening of an external charge in Coulomb systems, so this term was adopted also for dislocations. In the same work,[20] numerical results were presented, but because of the prohibitive fluctuations of the dislocation distribution induced by an external fixed dislocation, the signed pair correlation of dislocations in equilibrium was monitored. Even in the latter function, an agreement with the theory was found.

It should be borne in mind that the relation between the externally induced density (response function) and the correlation function is based on linear-response theory in thermal systems. However, in the dislocation system considered presently, entropic effects are suppressed, i.e., thermal fluctuations are negligible beside the Peach-Koehler forces. Therefore, traditional arguments of linear-response theory do not obviously apply. This raises the question, why then the externally induced dislocations obey properties similar to those of correlation functions. The problem can be actually posed in a broad sense, namely, to what extent the response function to an external particle and the two-particle correlation function in or off equilibrium are similar. The evolution equations for the one-point densities with some simplifying hypotheses are known,[8] and they have been linked to the variational approach by a phase field construction.[21] The evolution equations for the two-point correlation functions, however, could not be brought to any treatable form so far.

As a recent development, Vinogradov and Willis[22,23] published an evolution equation for the correlation function of long parallel screw dislocations with the same Burgers vectors. They even solved the resulting equation for the static case analytically. It was found, however, that the generalization of this result for the case of two possible Burgers vectors (positive and negative dislocations) or for edge dislocations leads to a solution not decaying at infinity, thus it cannot be correct physically.

In this paper, we investigate the evolution of correlation functions of long parallel edge dislocations with single slip. We start our analysis with the Bogoliubov-Born-Green-Kirkwood-Yvon (BBGKY) hierarchy, describing the evolution of dislocation many-body densities, which was derived earlier by Groma.[5] In contrast to the cluster approximation used by Vinogradov and Willis,[22,23] we apply the Kirkwood superposition approximation as a method to close the chain of equations. The resulting equations, when rewritten for appropriately introduced single-point fields, are similar to those describing the evolution of one-dislocation density functions in the presence of a single external dislocation. In fact, they become identical if the external perturbation is small enough, thus we arrive at the analog of linear-response theory in thermal systems, now obtained for density fields at zero temperature. It should be kept in mind, however, that the relation is now conditioned on the Kirkwood approximation for the two-point correlations. In order to test the extent of the analogy between the one- and two-point densities, we also performed extensive simulations. First, we compared the equilibrium distributions induced by the screened single external dislocation with the appropriate fields from the two-point correlations and found a quite satisfactory agreement. Second, the time evolutions of the two types of density fields were matched and again, close similarity was observed even before reaching equilibrium. This essentially demonstrates that the Kirkwood closure approximation was justified and the resulting equations indeed well describe the evolution of the correlation functions. We also analyze the cluster approximation of Vinogradov and Willis, adopted for edge dislocations, and show that it leads to a physically unacceptable result for the evolution equation of the correlation functions.

The paper is organized as follows: In Sec. II we derive the equations of motion for the two-point correlation functions and for the formally introduced, effectively one-point fields. Section III recuperates the equations for the single dislocation densities, while Sec. IV is devoted to the comparison of the previous two sections' results. Section V contains the presentation of the outcome of the simulations. The conclusions are followed by the Appendix, containing background calculations for Sec. II.

II. TIME EVOLUTION OF THE CORRELATION FUNCTIONS

Let us consider a system of parallel edge dislocations with single slip system, where only overdamped glide motion is allowed. By considering a cross section of the crystal perpendicular to the dislocations, the problem becomes two dimensional with pointlike objects. If s_i denotes the sign of the ith dislocation, then its Burgers vector is $\boldsymbol{b}_i = s_i \boldsymbol{b}$ $[s_i \in \{+,-\}$ and $\boldsymbol{b} := (b,0)]$. Let $\boldsymbol{r}_i(t)$ be the position and $\boldsymbol{v}_i(t)$ the velocity of the ith dislocation at time t. The equation of motion of the ith dislocation can then be written in the form,

$$\boldsymbol{v}_i(t) = B\left(\sum_{\substack{j=1\\ j\neq i}}^{N} s_j \boldsymbol{b}_i \tau_{\text{ind}}(\boldsymbol{r}_i(t) - \boldsymbol{r}_j(t)) + \boldsymbol{b}_i \tau_{\text{ext}}(\boldsymbol{r}_i(t))\right), \quad (1)$$

where B is the dislocation mobility, τ_{ind} is the shear stress field generated by a single edge dislocation positioned in the origin, and $\tau_{\text{ext}}(\boldsymbol{r})$ is an arbitrary spatially varying external stress field. In the studies presented in this paper, the medium is assumed to be isotropic; hence,

$$\tau_{\text{ind}}(\boldsymbol{r}) = \frac{\mu |\boldsymbol{b}|}{2\pi(1-\nu)} \frac{x(x^2-y^2)}{(x^2+y^2)^2}, \quad (2)$$

with μ and ν being the shear modulus and the Poisson's ratio, respectively. Since the value of the kinetic coefficient B only affects the time scale of dislocation motion, in the rest of this paper, it is absorbed into the time unit with the $t \to Bt$ substitution. The same could be done with the μ and ν material parameters, with the system size, and with the Burgers vector $|\boldsymbol{b}|$ (for details, see Sec. V).

In order to describe a discrete system of dislocations, it is useful to introduce discrete n-particle dislocation densities, e.g., $\rho_1^{D,s}(\boldsymbol{r},t) := \sum_{i=1}^{N} \delta_{s,s_i} \delta(\boldsymbol{r}-\boldsymbol{r}_i(t))$ for $n=1$ in a system of N dislocations (for details, see, e.g., Ref. 21). Here, with the superscript s we make a distinction between the densities of positive and negative dislocations. Higher-order discrete densities could be defined accordingly. In order to get smooth density functions, one has to perform averaging over statistically equivalent systems, which is denoted as, e.g., $\rho_1^s(\boldsymbol{r},t) := \langle \rho_1^{D,s}(\boldsymbol{r},t) \rangle$. After performing the averaging procedure, Groma[5] obtained a chain of evolution equations for the $\rho_n^{s_1,\ldots,s_n}$ n-particle density functions of the system. These equations give the rate change of $\rho_n^{s_1,\ldots,s_n}$, which depends on both itself and the one-level higher density function $\rho_{n+1}^{s_1,\ldots,s_{n+1}}$. This type of chain of equations is called BBGKY hierarchy in statistical physics. To make it possible to solve these infinite number of equations, the hierarchy must be chopped at a certain level.

We start our investigations at the first level of the hierarchy, which governs the evolution of the one-particle density functions:[5]

$$\frac{\partial \rho_1^{s_1}(\boldsymbol{r}_1,t)}{\partial t} + \frac{\partial}{\partial \boldsymbol{r}_1} \sum_{s_2=\pm 1} \int_{\mathbb{R}^2} \rho_2^{s_1,s_2}(\boldsymbol{r}_1,\boldsymbol{r}_2,t) \boldsymbol{F}^{s_1,s_2}(\boldsymbol{r}_1-\boldsymbol{r}_2) d^2 r_2 + \frac{\partial}{\partial \boldsymbol{r}_1}[\rho_1^{s_1}(\boldsymbol{r}_1,t)\boldsymbol{F}_{\text{ext}}^{s_1}(\boldsymbol{r}_1)] = 0, \tag{3}$$

where $\rho_n^{s_1,\ldots,s_n}$ denotes the n-particle dislocation density function with s_i referring to the sign of the ith dislocation, $\boldsymbol{F}^{s_1,s_2}(\boldsymbol{r}_1-\boldsymbol{r}_2)$ is the interaction force between two dislocations at positions $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$, and with signs s_1 and s_2 ($\boldsymbol{r}_i \in \mathbb{R}^2$),

$$\boldsymbol{F}^{s_1,s_2}(\boldsymbol{r}) = s_1 s_2 \tau_{\text{ind}}(\boldsymbol{r}) \boldsymbol{b}. \tag{4}$$

The $\tau_{\text{ext}}(\boldsymbol{r})$ spatially varying external shear stress results in the extra $\boldsymbol{F}_{\text{ext}}^{s}(\boldsymbol{r})$ force depending on the sign s,

$$\boldsymbol{F}_{\text{ext}}^{s}(\boldsymbol{r}) = s \tau_{\text{ext}}(\boldsymbol{r}) \boldsymbol{b}. \tag{5}$$

Solving Eq. (3) generally (with arbitrary boundary conditions) requires the additional knowledge of ρ_2.

In this section, we investigate the relaxation of dislocations from a random initial state in an infinite medium at zero external shear stress. Since the equations of motion of the dislocations do not have a direct spatial dependence, the system is invariant under translations. In this case, the system is homogeneous, meaning the one-particle density functions ρ_1^s cannot have a spatial dependence, i.e.,

$$\rho^{\pm} := \rho_1^{\pm}(\boldsymbol{r},t) = \text{const} \tag{6}$$

This is a trivial solution of Eq. (3). One can draw two simple conclusions from it:

(i) the two-particle density functions depend only on the difference of their arguments:

$$\rho_2^{s_1,s_2}(\boldsymbol{r}_1,\boldsymbol{r}_2,t) = \rho_2^{s_1,s_2}(\boldsymbol{r}_1-\boldsymbol{r}_2,t), \quad s_1,s_2 \in \{+,-\}, \tag{7}$$

(ii) and the following identity holds:

$$\sum_{s_2=\pm 1} s_2 \int_{\mathbb{R}^2} \rho_2^{s_1,s_2}(\boldsymbol{r},t) \tau_{\text{ind}}(\boldsymbol{r}) d^2 r = 0, \quad s_1 \in \{+,-\}. \tag{8}$$

We now proceed to the evolution equations of the two-particle density functions:[5]

$$\begin{aligned}
&\frac{\partial \rho_2^{s_1,s_2}(\boldsymbol{r}_1,\boldsymbol{r}_2,t)}{\partial t} + \left(\frac{\partial}{\partial \boldsymbol{r}_1} - \frac{\partial}{\partial \boldsymbol{r}_2}\right)[\rho_2^{s_1,s_2}(\boldsymbol{r}_1,\boldsymbol{r}_2,t)\boldsymbol{F}^{s_1,s_2}(\boldsymbol{r}_1-\boldsymbol{r}_2)] \\
&\quad + \frac{\partial}{\partial \boldsymbol{r}_1} \sum_{s_3=\pm 1} \int_{\mathbb{R}^2} \rho_3^{s_1,s_2,s_3}(\boldsymbol{r}_1,\boldsymbol{r}_2,\boldsymbol{r}_3,t)\boldsymbol{F}^{s_1,s_3}(\boldsymbol{r}_1-\boldsymbol{r}_3) d^2 r_3 \\
&\quad + \frac{\partial}{\partial \boldsymbol{r}_2} \sum_{s_3=\pm 1} \int_{\mathbb{R}^2} \rho_3^{s_1,s_2,s_3}(\boldsymbol{r}_1,\boldsymbol{r}_2,\boldsymbol{r}_3,t)\boldsymbol{F}^{s_2,s_3}(\boldsymbol{r}_2-\boldsymbol{r}_3) d^2 r_3 \\
&\quad + \frac{\partial}{\partial \boldsymbol{r}_1}[\rho_2^{s_1,s_2}(\boldsymbol{r}_1,\boldsymbol{r}_2,t)\boldsymbol{F}_{\text{ext}}^{s_1}(\boldsymbol{r}_1)] \\
&\quad + \frac{\partial}{\partial \boldsymbol{r}_2}[\rho_2^{s_1,s_2}(\boldsymbol{r}_1,\boldsymbol{r}_2,t)\boldsymbol{F}_{\text{ext}}^{s_2}(\mathbf{r}_2)] = 0.
\end{aligned} \tag{9}$$

It has to be noted that by definition $\rho_2^{s_1,s_2}(\boldsymbol{r}_1,\boldsymbol{r}_2,t) = \rho_2^{s_2,s_1}(\boldsymbol{r}_2,\boldsymbol{r}_1,t)$.

A possible method to truncate the hierarchy at this level is to express $\rho_3^{s_1,s_2,s_3}$ in the so-called cluster expansion and neglect the three-particle correlation term, as it was done by Groma,[5] and more recently by Vinogradov and Willis.[22,23] This means $\rho_3^{s_1,s_2,s_3}$ is approximated as

$$\begin{aligned}
\rho_3^{s_1,s_2,s_3}(\boldsymbol{r}_1,\boldsymbol{r}_2,\boldsymbol{r}_3,t) \approx{}& \rho_1^{s_1}(\boldsymbol{r}_1,t)\rho_1^{s_2}(\boldsymbol{r}_2,t)\rho_1^{s_3}(\boldsymbol{r}_3,t) \\
&\times[1 + d^{s_1,s_2}(\boldsymbol{r}_1,\boldsymbol{r}_2,t) + d^{s_2,s_3}(\boldsymbol{r}_2,\boldsymbol{r}_3,t) \\
&+ d^{s_3,s_1}(\boldsymbol{r}_3,\boldsymbol{r}_1,t)],
\end{aligned} \tag{10}$$

where the dislocation-dislocation correlation functions are defined in the usual way,

$$d^{s_1,s_2}(\boldsymbol{r}_1,\boldsymbol{r}_2,t) := \frac{\rho_2^{s_1,s_2}(\boldsymbol{r}_1,\boldsymbol{r}_2,t)}{\rho_1^{s_1}(\boldsymbol{r}_1,t)\rho_1^{s_2}(\boldsymbol{r}_2,t)} - 1. \tag{11}$$

Substituting the cluster expansion Eq. (10) into Eq. (9) leads to a closed evolution equation for $\rho_2^{s_1,s_2}$ or equivalently for d^{s_1,s_2}. Its steady-state solution was calculated by Vinogradov and Willis for infinite parallel screw dislocations.[22,23] Their motion was constrained to simply glide in one direction, so the difference between the system studied by them and the one considered in this paper is only the form of the generated stress field of the particles τ_{ind}. They derived an exact solution for the correlation function, when there were only positive screw dislocations. However, in the case when both positive and negative screw dislocations were present from the equation for the correlation functions, they deduced a mathematical contradiction. Namely, the correlation functions had to tend to a constant nonzero value for large distances, which is obviously incorrect for real dislocation arrangements. They also showed that this contradiction was independent from the actual form of τ_{ind}, which means that for edge dislocations, the equations are not solvable either. We thus speculate that according to this result, the cluster approximation is unphysical for the system of parallel edge dislocations.

Another traditional method for closing the hierarchy at this order is the Kirkwood superposition approximation,[24] which was successfully used, for instance, in fluid mechanics (for a brief overview, see, e.g., Ref. 25). In the context of dislocations, it was first introduced by Zaiser *et al.*;[7] but after investigating the resulting equations, only a few basic conclusions were drawn.

The Kirkwood superposition approximation expresses the three-particle density functions in terms of the pair densities,

$$\begin{aligned}\rho_3^{s_1,s_2,s_3}(\boldsymbol{r}_1,\boldsymbol{r}_2,\boldsymbol{r}_3,t) &\approx \frac{\rho_2^{s_1,s_2}(\boldsymbol{r}_1,\boldsymbol{r}_2,t)\rho_2^{s_2,s_3}(\boldsymbol{r}_2,\boldsymbol{r}_3,t)\rho_2^{s_3,s_1}(\boldsymbol{r}_3,\boldsymbol{r}_1,t)}{\rho_1^{s_1}(\boldsymbol{r}_1,t)\rho_1^{s_2}(\boldsymbol{r}_2,t)\rho_1^{s_3}(\boldsymbol{r}_3,t)}\\ &= \rho_1^{s_1}(\boldsymbol{r}_1,t)\rho_1^{s_2}(\boldsymbol{r}_2,t)\rho_1^{s_3}(\boldsymbol{r}_3,t)\\ &\quad\times[1+d^{s_1,s_2}(\boldsymbol{r}_1,\boldsymbol{r}_2,t)][1+d^{s_2,s_3}(\boldsymbol{r}_2,\boldsymbol{r}_3,t)]\\ &\quad\times[1+d^{s_3,s_1}(\boldsymbol{r}_3,\boldsymbol{r}_1,t)]. \end{aligned}\tag{12}$$

If we keep only the terms linear in the correlation functions d^{s_1,s_2}, this expression gives the same result as the "cluster approximation" [Eq. (10)]; i.e., their asymptotic behavior for large distances is identical. But as we will see, the nonlinear terms play an important role in the forthcoming derivation. We would like to emphasize that the Kirkwood factorization is indeed an approximation. For example, it does not fulfill the simple normalization condition that if the number of particles is finite (let us say N), then $\int_{\mathbb{R}^2}\rho_3(.,.,\boldsymbol{r},t)d^2r=(N-2)\rho_2$. Thus, it is expected that the superposition approximation cannot give precise results for small distances.

In the following, we continue with substituting the Kirkwood approximation [Eq. (12)] into the second-order evolution equation given by Eq. (9). According to the previous results for the studied homogeneous system [Eqs. (6) and (7)], the second term of Eq. (9) simplifies to

$$\begin{aligned}&\left(\frac{\partial}{\partial \boldsymbol{r}_1}-\frac{\partial}{\partial \boldsymbol{r}_2}\right)[\rho_2^{s_1,s_2}(\boldsymbol{r}_1,\boldsymbol{r}_2,t)\boldsymbol{F}^{s_1,s_2}(\boldsymbol{r}_1-\boldsymbol{r}_2)]\\ &\quad= 2s_1s_2\frac{\partial}{\partial \boldsymbol{r}_1}[\boldsymbol{b}\rho_2^{s_1,s_2}(\boldsymbol{r}_1-\boldsymbol{r}_2,t)\tau_{\text{ind}}(\boldsymbol{r}_1-\boldsymbol{r}_2)]. \end{aligned}\tag{13}$$

For the third and the fourth terms of Eq. (9), one gets

$$\begin{aligned}&\frac{\partial}{\partial \boldsymbol{r}_1}\sum_{s_3=\pm 1}\int_{\mathbb{R}^2}\rho_3^{s_1,s_2,s_3}(\boldsymbol{r}_1,\boldsymbol{r}_2,\boldsymbol{r}_3,t)\boldsymbol{F}^{s_1,s_3}(\boldsymbol{r}_1-\boldsymbol{r}_3)d^2r_3\\ &= \frac{s_1}{\rho^{s_1}\rho^{s_2}}\frac{\partial}{\partial \boldsymbol{r}_1}\Bigg[\boldsymbol{b}\rho_2^{s_1,s_2}(\boldsymbol{r}_1-\boldsymbol{r}_2,t)\sum_{s_3=\pm 1}\frac{s_3}{\rho^{s_3}}\\ &\times\int_{\mathbb{R}^2}\rho_2^{s_2,s_3}(-\boldsymbol{r}_3,t)\rho_2^{s_3,s_1}(\boldsymbol{r}_3-\boldsymbol{r}_1+\boldsymbol{r}_2,t)\\ &\times\tau_{\text{ind}}(\boldsymbol{r}_1-\boldsymbol{r}_2-\boldsymbol{r}_3)d^2r_3\Bigg], \end{aligned}\tag{14}$$

and

$$\begin{aligned}&\frac{\partial}{\partial \boldsymbol{r}_2}\sum_{s_3=\pm 1}\int_{\mathbb{R}^2}\rho_3^{s_1,s_2,s_3}(\boldsymbol{r}_1,\boldsymbol{r}_2,\boldsymbol{r}_3,t)\boldsymbol{F}^{s_2,s_3}(\boldsymbol{r}_2-\boldsymbol{r}_3)d^2r_3\\ &= -\frac{s_2}{\rho^{s_1}\rho^{s_2}}\frac{\partial}{\partial \boldsymbol{r}_2}\Bigg[\boldsymbol{b}\rho_2^{s_1,s_2}(\boldsymbol{r}_1-\boldsymbol{r}_2,t)\sum_{s_3=\pm 1}\frac{s_3}{\rho^{s_3}}\\ &\times\int_{\mathbb{R}^2}\rho_2^{s_2,s_3}(\boldsymbol{r}_3-\boldsymbol{r}_1+\boldsymbol{r}_2,t)\rho_2^{s_3,s_1}(-\boldsymbol{r}_3,t)\\ &\times\tau_{\text{ind}}(\boldsymbol{r}_1-\boldsymbol{r}_2-\boldsymbol{r}_3)d^2r_3\Bigg], \end{aligned}\tag{15}$$

where we also applied the $\tau_{\text{ind}}(-\boldsymbol{r})=-\tau_{\text{ind}}(\boldsymbol{r})$ relation. Finally, after introducing $\boldsymbol{r}:=\boldsymbol{r}_1-\boldsymbol{r}_2$ for the evolution equations of the second order, one arrives at

$$\begin{aligned}&\frac{\partial\rho_2^{s_1,s_2}(\boldsymbol{r},t)}{\partial t}+\frac{\partial}{\partial \boldsymbol{r}}\Bigg\{\Bigg[\boldsymbol{b}\rho_2^{s_1,s_2}(\boldsymbol{r},t)2s_1s_2\tau_{\text{ind}}(\boldsymbol{r})+(s_1-s_2)\tau_{\text{ext}}\\ &+\frac{1}{\rho^{s_1}\rho^{s_2}}\sum_{s_3=\pm 1}\frac{s_3}{\rho^{s_3}}\int_{\mathbb{R}^2}(s_1\rho_2^{s_3,s_2}(\boldsymbol{r}_3,t)\rho_2^{s_1,s_3}(\boldsymbol{r}-\boldsymbol{r}_3,t)\\ &+s_2\rho_2^{s_1,s_3}(\boldsymbol{r}_3,t)\rho_2^{s_3,s_2}(\boldsymbol{r}-\boldsymbol{r}_3,t))\tau_{\text{ind}}(\boldsymbol{r}-\boldsymbol{r}_3)d^2r_3\Bigg]\Bigg\}=0. \end{aligned}\tag{16}$$

The correlation functions defined by Eq. (11) due to Eqs. (6) and (7) are simplified to

$$d^{s_1,s_2}(\boldsymbol{r},t)=\frac{\rho_2^{s_1,s_2}(\boldsymbol{r},t)}{\rho^{s_1}\rho^{s_2}}-1. \tag{17}$$

By substituting Eq. (17) into Eq. (16), one gets a closed set of equations for the two-particle correlation functions d^{s_1,s_2}.

In the rest of this paper, it is assumed that:

(i) the number of positive and negative signed dislocations are equal ($\rho^+=\rho^-$).

(ii) the external shear stress is zero ($\tau_{\text{ext}}=0$).

As it is explained in details in the Appendix, it follows that $d^{++}(\boldsymbol{r},t)=d^{--}(\boldsymbol{r},t)$ and $d^{+-}(\boldsymbol{r},t)=d^{-+}(\boldsymbol{r},t)$ for every $\boldsymbol{r}$ and t, meaning there are only two independent correlation functions: d^{++} and d^{+-}. Under these conditions, the evolution equations are simplified to (for details, see the Appendix)

$$\partial_t d^{++}+2\nabla[\boldsymbol{b}(1+d^{++})(\tau_{\text{ind}}+\tau_{\text{sc}}^h+\tau_b^h+\tau_a^h)]=0, \tag{18}$$

$$\partial_t d^{+-}+2\nabla[\boldsymbol{b}(1+d^{+-})(-\tau_{\text{ind}}-\tau_{\text{sc}}^h-\tau_b^h+\tau_a^h)]=0, \tag{19}$$

where we have introduced the following terms having stress dimension:

$$\tau_{\text{sc}}^h(\boldsymbol{r},t):=\rho^+\int_{\mathbb{R}^2}2d_d(\boldsymbol{r}',t)\tau_{\text{ind}}(\boldsymbol{r}-\boldsymbol{r}')d^2r', \tag{20}$$

$$\tau_b^h(\boldsymbol{r},t):=\rho^+\int_{\mathbb{R}^2}2d_d(\boldsymbol{r}',t)d_s(\boldsymbol{r}-\boldsymbol{r}',t)\tau_{\text{ind}}(\boldsymbol{r}-\boldsymbol{r}')d^2r', \tag{21}$$

$$\tau_a^h(\boldsymbol{r},t) \coloneqq \rho^+ \int_{\mathbb{R}^2} 2d_s(\boldsymbol{r}',t)d_d(\boldsymbol{r}-\boldsymbol{r}',t)\tau_{\text{ind}}(\boldsymbol{r}-\boldsymbol{r}')d^2r', \tag{22}$$

with $d_s \coloneqq (d^{++}+d^{+-})/2$ and $d_d \coloneqq (d^{++}-d^{+-})/2$.

Dislocations of opposite signs should move at each given point with equal velocities but in opposite directions, which implies

$$\tau_a^h(\boldsymbol{r},t) = 0, \tag{23}$$

for every $\boldsymbol{r}$ and t. This argument is identical to that of the Appendix of Ref. 8, where a similar stress term is omitted.

The final evolution Eqs. (18) and (19) with Eq. (23) are very similar to those obtained by Groma *et al.*[8] for the one-particle dislocation densities. To emphasize the analogy even more, let us introduce the following notations:

$$\rho^h(\boldsymbol{r},t) \coloneqq \rho^+[2 + d^{++}(\boldsymbol{r},t) + d^{+-}(\boldsymbol{r},t)] = 2\rho^+[1 + d_s(\boldsymbol{r},t)], \tag{24}$$

$$\kappa^h(\boldsymbol{r},t) \coloneqq \rho^+[d^{++}(\boldsymbol{r},t) - d^{+-}(\boldsymbol{r},t)] = 2\rho^+ d_d(\boldsymbol{r},t). \tag{25}$$

(Here and previously, the "h" superscript refers to the homogeneous system.) Although these quantities have density dimensions, they are auxiliary quantities and do not carry the meaning of single-particle densities. The evolution equations for these newly introduced quantities can be written as

$$\partial_t \rho^h + 2\,\nabla\,[\boldsymbol{b}\kappa^h(\tau_{\text{ind}} + \tau_{\text{sc}}^h + \tau_b^h)] = 0, \tag{26}$$

$$\partial_t \kappa^h + 2\,\nabla\,[\boldsymbol{b}\rho^h(\tau_{\text{ind}} + \tau_{\text{sc}}^h + \tau_b^h)] = 0, \tag{27}$$

with

$$\tau_{\text{sc}}^h(\boldsymbol{r},t) = \int_{\mathbb{R}^2} \kappa^h(\boldsymbol{r}',t)\tau_{\text{ind}}(\boldsymbol{r}-\boldsymbol{r}')d^2r', \tag{28}$$

$$\tau_b^h(\boldsymbol{r},t) = \int_{\mathbb{R}^2} \kappa^h(\boldsymbol{r}',t)d_s(\boldsymbol{r}-\boldsymbol{r}',t)\tau_{\text{ind}}(\boldsymbol{r}-\boldsymbol{r}')d^2r'. \tag{29}$$

These are the equations that govern the evolution of dislocation-dislocation correlation functions. Instead of their numerical solution, we will prove their correctness by an analogy with the phenomena of screening of an individual dislocation, which is discussed in Sec. III.

III. DISLOCATION DENSITY FIELDS OF A SCREENED EXTERNAL DISLOCATION

The stress field of a single dislocation decays as $1/r$. This implies that if the distribution of the dislocations was completely random in a crystal, then the elastic energy per unit volume would diverge logarithmically with the crystal size.[26] Since this cannot be observed in real systems, the only possible solution is that dislocations arrange themselves in a correlated way, which screens out their long-range effect. The phenomenon lends itself to the analogy with Debye screening in Coulomb systems.

In order to address the problem, Groma *et al.*[20,21] studied the induced geometrically necessary dislocation density around a single external edge dislocation in 2D, proposed an equation for the stress potential in equilibrium, and gave analytic solution for the infinite plane—provided the total density was constant and much larger than the geometrically necessary dislocation density. While this is not the original question of the correlation function, within linear-response theory, however, the result is expected to be valid also to the correlation problem. It was indeed shown that the screened dislocation's stress field decays faster than that of the unscreened ones, in the direction perpendicular to the Burgers vector by a power law and in all other directions exponentially. This result was actually compared to correlation simulations, mostly because this was numerically simpler than the computation of the induced field by an external dislocation, and in the direction of the power decay, not only the exponent but the entire shape predicted by theory was recovered in the simulation. However, the exponential decay along the x axis was not seen as in the theoretical solution, mostly because of the special conditions of dislocation motion on a torus as realized in the simulation. In any event, the equivalence of response to an external dislocation and the correlation in the absence of a fixed external one was taken for granted; precisely the problem addressed in the present paper.

An important peculiar aspect of screening of dislocations has to be emphasized. First, we recall that in a thermal system like Coulomb plasma linear-response theory provides enough ground to expect the similarity between screening of an external charge and that in the correlation. On the other hand, the screening problem of dislocations already emerges at zero physical temperature. Now the role of the temperature in keeping oppositely charged particles at a distance is taken over by the constraint to slip axes, so here, an effective temperature parameter arises that can be determined from comparison with simulation.[20,21] Now given the fact that we only have a temperature parameter (which directly appears in the effective thermodynamic potential) but not usual thermodynamics, it is by far not obvious that the two types of screening, namely, the one of an external dislocation, and the one appearing in the correlation function, should maintain the same type of equivalence as if Boltzmannian thermodynamics were valid. Hence, in the case of dislocations, it remains an open problem what the relation is between screening by response to an external effect and screening in the correlations.

In Sec. II, we constructed the equations of motion for correlations, now we do the same for the one-particle densities in the presence of an external dislocation. As a result of the stress field generated by the inserted object, the positions of the other dislocations change and a new relaxed state evolves. In it for instance, one-particle dislocation densities will not be constant any more. In this section, the time evolution of these functions is investigated.

Due to the spatially varying extra force acting on the dislocations, the system is not translation invariant any more. So, in the case of screening an external dislocation, contrary to the case in Sec. II, the system is spatially inhomogeneous. The evolution of the one-particle densities is described by the first member of the BBGKY hierarchy [Eq. (3)],

$$\frac{\partial \rho_1^{s_1}(\boldsymbol{r}_1,t)}{\partial t} + \frac{\partial}{\partial \boldsymbol{r}_1}\sum_{s_2=\pm 1}\int_{\mathbb{R}^2}\rho_2^{s_1,s_2}(\boldsymbol{r}_1,\boldsymbol{r}_2,t)\boldsymbol{F}^{s_1,s_2}(\boldsymbol{r}_1-\boldsymbol{r}_2)d^2r_2 + \frac{\partial}{\partial \boldsymbol{r}_1}[\rho_1^{s_1}(\boldsymbol{r}_1,t)\boldsymbol{F}_{\text{scr}}^{s_1}(\boldsymbol{r}_1)] = 0, \tag{30}$$

where we introduced the notation $\boldsymbol{F}_{\text{scr}}^{s}(\boldsymbol{r}) \coloneqq sb\boldsymbol{b}\tau_{\text{ind}}(\boldsymbol{r})$ with $b \coloneqq |\boldsymbol{b}|$ for the stress field of the extra dislocation.

According to the deduction in Ref. 8, Eq. (30) can be cast into the following form:

$$\partial_t\rho + \nabla[\boldsymbol{b}\kappa(\tau_{\text{ind}} + \tau_{\text{sc}} - \tau_f + \tau_b)] = 0, \tag{31}$$

$$\partial_t\kappa + \nabla[\boldsymbol{b}\rho(\tau_{\text{ind}} + \tau_{\text{sc}} - \tau_f + \tau_b)] = 0, \tag{32}$$

where we have introduced the

$$\rho(\boldsymbol{r},t) \coloneqq \rho^+(\boldsymbol{r},t) + \rho^-(\boldsymbol{r},t) \tag{33}$$

and

$$\kappa(\boldsymbol{r},t) \coloneqq \rho^+(\boldsymbol{r},t) - \rho^-(\boldsymbol{r},t), \tag{34}$$

total and geometrically necessary dislocation densities, respectively, and

$$\tau_{\text{sc}}(\boldsymbol{r},t) \coloneqq \int_{\mathbb{R}^2}\kappa(\boldsymbol{r}',t)\tau_{\text{ind}}(\boldsymbol{r}-\boldsymbol{r}')d^2r', \tag{35}$$

$$\tau_b(\boldsymbol{r},t) \coloneqq \int_{\mathbb{R}^2}\kappa(\boldsymbol{r}',t)\tilde{d}(\boldsymbol{r},\boldsymbol{r}',t)\tau_{\text{ind}}(\boldsymbol{r}-\boldsymbol{r}')d^2r', \tag{36}$$

$$\tau_f(\boldsymbol{r},t) \coloneqq \frac{1}{2}\int_{\mathbb{R}^2}\rho(\boldsymbol{r}',t)\tilde{d}_a(\boldsymbol{r},\boldsymbol{r}',t)\tau_{\text{ind}}(\boldsymbol{r}-\boldsymbol{r}')d^2r', \tag{37}$$

with $\tilde{d} \coloneqq (\tilde{d}^{++}+\tilde{d}^{--}+\tilde{d}^{+-}+\tilde{d}^{-+})/4$ and $\tilde{d}_a \coloneqq (\tilde{d}^{+-}-\tilde{d}^{-+})/2$. We note that in this inhomogeneous case, the correlation functions do not depend on the difference of their arguments, meaning one has to remain at the general definition [Eq. (11)]. Here and in the rest of this paper, $\widetilde{(\cdot)}$ indicates that the correlation function has two spatial variables. During the derivation of Eqs. (31) and (32), no approximations have been made.

If the correlation functions were short range, it could be approximated that they depend only on the relative coordinate $\boldsymbol{r}_1-\boldsymbol{r}_2$,

$$\rho_2^{s_1,s_2}(\boldsymbol{r}_1,\boldsymbol{r}_2,t) = \rho_1^{s_1}(\boldsymbol{r}_1,t)\rho_1^{s_2}(\boldsymbol{r}_2,t)[1 + d^{s_1,s_2}(\boldsymbol{r}_1-\boldsymbol{r}_2,t)]. \tag{38}$$

Here, the correlation function d^{s_1,s_2} can be taken from homogeneous systems.[8] The assumed shortness of dislocation-dislocation correlations was proved on discrete dislocation simulation results earlier.[7] It was found that the correlation functions decay to zero exponentially within a few average dislocation spacings.

Because of the short-range nature of dislocation-dislocation correlations, the κ and ρ functions can be approximated by their Taylor expansions in the integrals of Eqs. (36) and (37). After keeping only the first nonvanishing terms, Groma *et al.* arrived at

$$\tau_b(\boldsymbol{r},t) = -\frac{\mu}{2\pi(1-\nu)}D_d\frac{b}{\rho(\boldsymbol{r},t)}\partial_x\kappa(\boldsymbol{r},t) \tag{39}$$

and

$$\tau_f(\boldsymbol{r},t) = \frac{\mu}{4\pi(1-\nu)}C_d b\sqrt{\rho(\boldsymbol{r},t)}, \tag{40}$$

where D_d and C_d are positive constants.[8] The term τ_b is a gradientlike contribution to the stress and is called "back stress," while τ_f can be interpreted as a local flow stress. The physical correctness of these approximations was proved by discrete dislocation simulations.[8–10]

The description of Debye screening of an external dislocations was based on a thermodynamic potential-like functional from which the evolution Eqs. (31) and (32) for κ and ρ can be derived.[20,21] In it, τ_b is approximated as in Eq. (39) and τ_f is omitted. In the case of ρ=const, the analytical solution of the static case was given and compared to numerical simulations.[20]

In what follows, we shall see that to establish the connection between the evolution of correlation functions and the screening field of a single external dislocations, we will not need the approximations in Eqs. (38)–(40) for the correlation functions τ_b and τ_f, respectively, rather will keep the more general definitions in Eqs. (36) and (37).

IV. CONNECTION BETWEEN THE SCREENED DISLOCATION DENSITIES AND THE CORRELATION FUNCTIONS

In Secs. II and III, we have derived evolution equations for correlation functions in a homogeneous system within the Kirkwood approximation, as well as for induced dislocation densities around a fixed external dislocation. The main message of this paper is that the deduced equations for the two different cases, namely, Eqs. (24) and (25) and Eqs. (31) and (32) are very similar. More is true, however, they become identical if special equalities hold for various *d*-*s* and time is appropriately rescaled. In detail, these conditions are the following:

(i) if the numbers of + and − dislocations are the same, then in the absence of external stresses, $d^{+-}(\boldsymbol{r},t)=d^{-+}(\boldsymbol{r},t)$ and $d^{++}(\boldsymbol{r},t)=d^{--}(\boldsymbol{r},t)$. So, if the general correlation functions are approximated by the ones taken from homogeneous systems, i.e.,

$$\tilde{d}^{s_1,s_2}(\boldsymbol{r}_1,\boldsymbol{r}_2,t) = d^{s_1,s_2}(\boldsymbol{r}_1-\boldsymbol{r}_2,t), \tag{41}$$

(ii) then $\tilde{d}_a(\boldsymbol{r}_1,\boldsymbol{r}_2,t)=0$ and $\tilde{d}(\boldsymbol{r}_1,\boldsymbol{r}_2,t)=d_s(\boldsymbol{r}_1-\boldsymbol{r}_2,t)$. In this case, the "flow-stress" term τ_f disappears from Eqs. (31) and (32), while it was never present in Eqs. (24) and (25). Moreover, the τ_b in Eqs. (31) and (32) becomes equal to the τ_b^h of Eqs. (24) and (25).

The main theoretical result of this paper immediately follows: namely, if one takes a solution of Eqs. (24) and (25) *for* $d^{++}(\boldsymbol{r},t)$ *and* $d^{+-}(\boldsymbol{r},t)$, next substitutes these into Eqs. (31) and (32), then the latter equations will have a solution identical to the one in Eqs. (24) and (25).

Physically, the equality $\tilde{d}(\boldsymbol{r}_1,\boldsymbol{r}_2,t)=d_s(\boldsymbol{r}_1-\boldsymbol{r}_2,t)$ corresponds to the approximation when the effect of the stress by

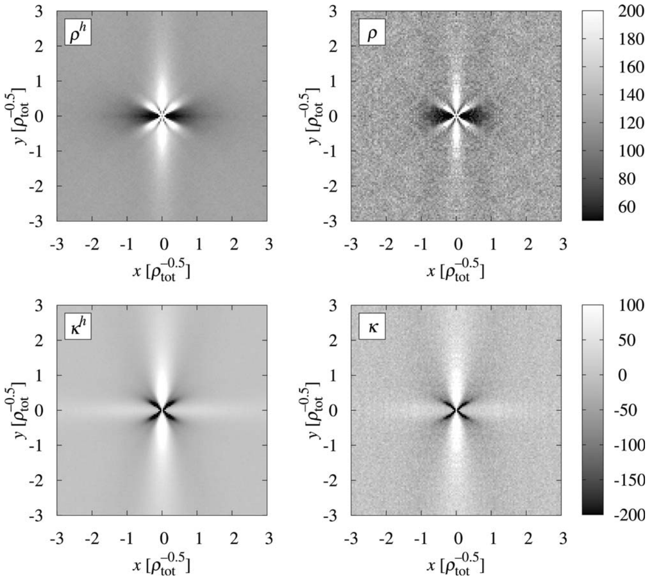

FIG. 1. The ρ^h, ρ, κ^h, and κ functions in the relaxed state obtained from numerical simulations. The distances are measured in $\rho_{\mathrm{tot}}^{-0.5}$ average dislocation spacings, where $\rho_{\mathrm{tot}} := \rho^+ + \rho^-$ is the total dislocation density.

the external dislocation in Eqs. (31) and (32) are neglected in the correlation functions. This condition amounts to taking the external effect as a first-order perturbation, in perfect analogy of linear-response theory valid for conventional thermal systems.

The divergencelike terms in Eqs. (24) and (25) are multiplied by two, which only affects the time scale of the process. The appearance of this factor can be well understood if we consider two dislocations moving in each others' stress fields. They relax into the same configuration, either we keep the position of the first dislocation fixed or not. The only difference is that the relaxation in the first case (which corresponds to screening of an individual dislocation) lasts twice as long as in the case, when both dislocations can glide freely (the case of the evolution of correlation functions).

To sum up, since at $t=0$, $\rho(\boldsymbol{r},0)=\rho^h(\boldsymbol{r},0)=\rho^+ + \rho^-$ and $\kappa(\boldsymbol{r},0)=\kappa^h(\boldsymbol{r},0)=0$, it follows that

$$\rho(\boldsymbol{r},2t) = \rho^h(\boldsymbol{r},t) = \rho^+[2 + d^{++}(\boldsymbol{r},t) + d^{+-}(\boldsymbol{r},t)], \tag{42}$$

and

$$\kappa(\boldsymbol{r},2t) = \kappa^h(\boldsymbol{r},t) = \rho^+[d^{++}(\boldsymbol{r},t) - d^{+-}(\boldsymbol{r},t)], \tag{43}$$

for every $\boldsymbol{r}$ and t. We would like to stress that during the derivation of this statement, we made approximations for both (ρ^h, κ^h) and for (ρ, κ) functions. For the first set, the Kirkwood superposition approximation [Eq. (12)], and for the second linear response was assumed; meaning general correlation functions were approximated by the ones taken from infinite homogeneous systems [Eq. (41)]. If the comparison of the numerically obtained functions confirms the validity of Eqs. (42) and (43), then it would also confirm the applicability of the Kirkwood superposition approximation. In Sec. V, this comparison is discussed.

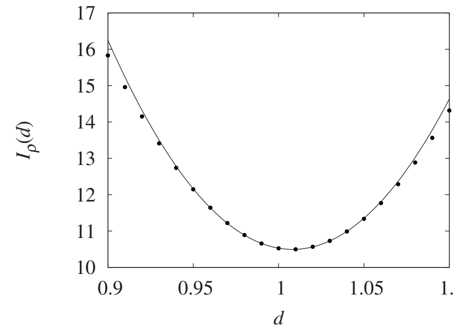

FIG. 2. The I_ρ function calculated numerically at different values (data points). A second-order polynomial was fitted around the minimum of the points (solid line).

V. SIMULATION RESULTS

To measure ρ^h, ρ, κ^h, and κ numerically, we first performed more than 13 000 different relaxations. In each of them at the beginning, 128 dislocations (64 with positive and 64 with negative sign) were distributed randomly in an $L \times L$ squarelike domain with periodic boundary conditions, and then they relaxed to a steady state. The d^{++} and d^{+-} correlation functions and the ρ^h and κ^h quantities were determined from these configurations by counting the relative coordinates of the dislocations. They are plotted in the first column of Fig. 1.

Afterwards, a new dislocation with positive sign was placed at the center of the simulation area in each configuration, and the systems were left to relax again, while the extra dislocation was fixed. These simulations correspond to the phenomena of Debye screening of an external dislocation. The ρ^+ and ρ^- densities were obtained by counting the number of positive and negative dislocations falling into each cell of a 256×256 mesh. Then ρ and κ functions defined in Eqs. (33) and (34) were calculated. They are also plotted in Fig. 1.

The two functions, according to our expectations are quite similar. The difference is that in the case of κ and ρ, the amplitude of the noise is much higher. The simple reason for this is that a relaxed system of N dislocations gives $N(N-1)$ data (the relative coordinates) during the calculation of the correlation functions, but only N data (the positions) when calculating the densities. In order to make a comparison between these functions, the following function was considered:

$$I_\rho(d) := \int_A |\rho(\boldsymbol{r}) - d\rho^h(\boldsymbol{r})| \, d^2 r. \tag{44}$$

The integral of a noise is nearly constant, so if ρ and ρ^h are equal except for the noise, then this quantity must have a minimum at $d=1$. As it was mentioned in Sec. II, the Kirkwood superposition approximation is not expected to be correct for distances smaller than an average dislocation spacing, and so, Eqs. (42) and (43) should apply only for $r=|\boldsymbol{r}| \gtrsim \rho_{\mathrm{tot}}^{-0.5}$ ($\rho_{\mathrm{tot}} := \rho^+ + \rho^-$ and $\rho_{\mathrm{tot}}^{-0.5}$ is the average dislocation

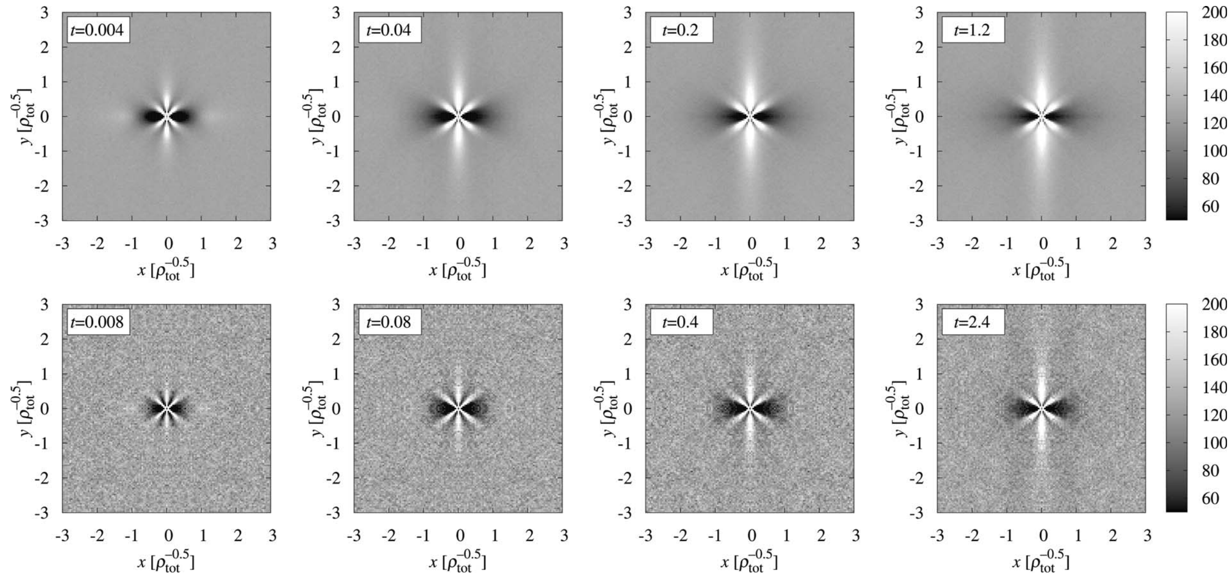

FIG. 3. The evolution of ρ^h (first row) and ρ (second row). The time t is measured in $\frac{2\pi(1-\nu)L^2}{b^2\mu B}$ dimensionless units. According to Eq. (42), $\rho^h(\boldsymbol{r},t)$ and $\rho(\boldsymbol{r},2t)$ are compared.

spacing). Accordingly, it is meaningful to define the domain of the integration A so that a circle of radius $0.5\rho_{\rm tot}^{-0.5}$ around the origin is left out from it. The numerically obtained function I_ρ is plotted in Fig. 2. As it can be seen, I_ρ indeed has a minimum around $d=1$. This confirms that the ρ^h and ρ functions can be considered equal in first approximation. The repetition of this calculation for κ^h and κ leads to similar results.

In Fig. 3, ρ^h and ρ functions can be seen at different times obtained from the numerical simulations. According to Eq. (42), $\rho^h(\boldsymbol{r},t)$ was compared to $\rho(\boldsymbol{r},2t)$ because of the factor of two appearing in the evolution equations of the correlation functions in Eqs. (26) and (27). The same can be seen for the κ functions in Fig. 4. To summarize, it can be stated that Eqs. (42) and (43) are at least in first order, fulfilled.

VI. CONCLUSIONS

In this paper, we derived evolution equations for the correlation functions of long parallel edge dislocations. We started our analysis at the BBGKY hierarchy of dislocation many-body densities, which was deduced earlier from the equations of motion of individual dislocations.[5] As a closure approximation for the hierarchy, the Kirkwood superposition approximation was used. Our investigations showed that the evolution of the correlation functions and the dislocation

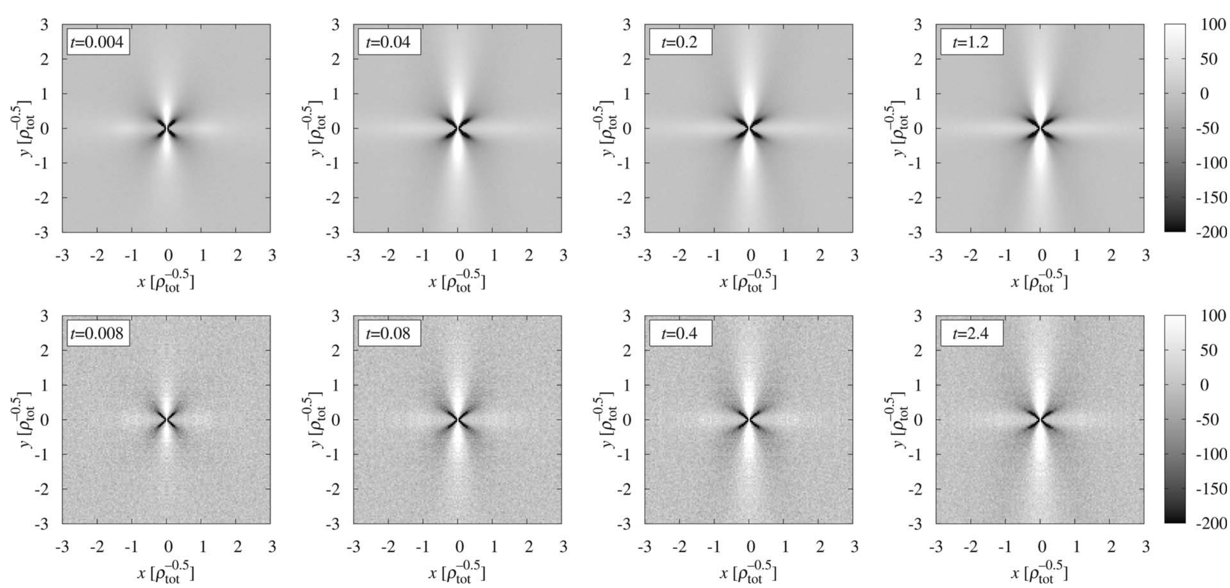

FIG. 4. The evolution of κ^h (first row) and κ (second row). The time t is measured in $\frac{2\pi(1-\nu)L^2}{b^2\mu B}$ dimensionless units. According to Eq. (43), $\kappa^h(\boldsymbol{r},t)$ and $\kappa(\boldsymbol{r},2t)$ are compared.

density fields evolving around a screened dislocation are closely related [according to Eqs. (42) and (43), only the time scale of the processes is different]. In Sec. V, this statement was confirmed by the numerical simulation.

The Kirkwood superposition approximation [Eq. (12)] gives the three-particle dislocation density in terms of the pair correlations. Contrary to the cluster approximation [Eq. (10)], it contains quadratic and cubic terms of the correlation function beside the linear one. As it was mentioned in Sec. II, these higher-order terms play an important role. According to our analysis presented in this paper, the omission of the cubic term leads to the disappearance of the back-stress term τ_b^h in the evolution Eqs. (26) and (27). This corresponds to the mean-field approximation, where dislocation correlations are neglected, resulting in the stress acting on dislocations is simply the self-consistent field τ_{sc}^h (Refs. 5 and 6)

If one neglects the cubic and quadratic terms (which is the cluster approximation), not only the back stress τ_b^h but also the self-consistent field τ_{sc}^h disappears, which is obviously unphysical. We mentioned in Sec. II that the cluster approximation [Eq. (10)] used by Vinogradov and Willis leads to a mathematical contradiction in the case of edge dislocations of opposite signs.[22,23] This result is in complete agreement with our analysis.

The Kirkwood superposition approximation leads to the evolution Eqs. (26) and (27). Their correctness was proved implicitly by the facts that: (i) analogy was found with the one-particle density evolution equations and (ii) the numerical work confirmed the similitude between the evolution of the one- and two-particle distributions. The authors believe that the obtained results may be valid for different forms of the interaction force τ_{ind}, e.g., for dislocations in anisotropic medium or for screw dislocations, even for other systems.

Another way of testing the deduced integrodifferential evolution equations could be their numerical solution. This is out of the scope of the present paper and requires further numerical work.

ACKNOWLEDGMENTS

The financial support of the Hungarian Scientific Research Fund (OTKA) under Contract No. K 67778, and of the European Community's Human Potential Programme under Contract No. NMP3-CT-2006-017105 [DIGIMAT] are gratefully acknowledged.

APPENDIX

In this section, we derive evolution equations for the correlation functions [which were defined by Eq. (11)] starting from the evolution Eq. (16) of $\rho_2^{s_1,s_2}$. First, we assume that the densities of positive and negative dislocations are equal ($\rho^+=\rho^-$). It can be noted that in this case, if $\rho_2^{++}(\boldsymbol{r},t)=\rho_2^{--}(\boldsymbol{r},t)$ for any t, then the second term of Eq. (16) is equal for both ρ_2^{++} and ρ_2^{--}. This means that the evolutions of ρ_2^{++} and ρ_2^{--} are identical; hence, $\rho_2^{++}(\boldsymbol{r},t)=\rho_2^{--}(\boldsymbol{r},t)$ and therefore, $d^{++}(\boldsymbol{r},t)=d^{--}(\boldsymbol{r},t)$ for every t. For this reason, one has to deal only with d^{++}, d^{+-}, and d^{-+}. Let us introduce

$$d_p := (d^{+-}+d^{-+})/2, \tag{A1}$$

and

$$d_a := (d^{+-}-d^{-+})/2, \tag{A2}$$

namely, the symmetric and the antisymmetric part of d^{+-}. Furthermore, we define d_s and d_d as the half of the sum and the difference of d^{++} and d_p, respectively,

$$d_s := (d^{++}+d_p)/2, \tag{A3}$$

and

$$d_d := (d^{++}-d_p)/2. \tag{A4}$$

It is also useful to introduce the following quantities having stress dimensions:

$$\tau_{\mathrm{sc}}^h(\boldsymbol{r},t) := \rho^+\int_{\mathbb{R}^2} 2d_d(\boldsymbol{r}',t)\tau_{\mathrm{ind}}(\boldsymbol{r}-\boldsymbol{r}')d^2r', \tag{A5}$$

$$\tau_b^h(\boldsymbol{r},t) := \rho^+\int_{\mathbb{R}^2} 2d_d(\boldsymbol{r}',t)d_s(\boldsymbol{r}-\boldsymbol{r}',t)\tau_{\mathrm{ind}}(\boldsymbol{r}-\boldsymbol{r}')d^2r', \tag{A6}$$

$$\tau_f^h(\boldsymbol{r},t) := -\frac{1}{2}\rho^+\int_{\mathbb{R}^2} d_a(\boldsymbol{r}',t)d_a(\boldsymbol{r}-\boldsymbol{r}',t)\tau_{\mathrm{ind}}(\boldsymbol{r}-\boldsymbol{r}')d^2r', \tag{A7}$$

$$\tau_a^h(\boldsymbol{r},t) := \rho^+\int_{\mathbb{R}^2}\left[2d_s(\boldsymbol{r}',t)d_d(\boldsymbol{r}-\boldsymbol{r}',t) + \frac{1}{2}d_a(\mathbf{r}',t)d_a(\boldsymbol{r}-\boldsymbol{r}',t)\right]\tau_{\mathrm{ind}}(\boldsymbol{r}-\boldsymbol{r}')d^2r', \tag{A8}$$

$$\tau_p^h(\boldsymbol{r},t) := \rho^+\int_{\mathbb{R}^2}\{d_a(\boldsymbol{r}',t)[1+d^{++}(\boldsymbol{r}-\boldsymbol{r}',t)] - [1+d^{++}(\boldsymbol{r}',t)]d_a(\boldsymbol{r}-\boldsymbol{r}',t)\}\tau_{\mathrm{ind}}(\boldsymbol{r}-\boldsymbol{r}')d^2r'. \tag{A9}$$

With these new functions from the evolution Eq. (16) for the correlation functions, one obtains

$$\partial_t d^{++} + 2\nabla[\boldsymbol{b}(1+d^{++})(\tau_{\mathrm{ind}}+\tau_{\mathrm{sc}}^h+\tau_b^h-\tau_f^h+\tau_a^h)]=0, \tag{A10}$$

$$\partial_t d^{+-} + 2\nabla[\boldsymbol{b}(1+d^{+-})(-\tau_{\mathrm{ind}}+\tau_{\mathrm{ext}}-\tau_{\mathrm{sc}}^h-\tau_b^h+\tau_f^h+\tau_a^h+\tau_p^h)] = 0, \tag{A11}$$

$$\partial_t d^{-+} + 2\nabla[\boldsymbol{b}(1+d^{-+})(-\tau_{\mathrm{ind}}-\tau_{\mathrm{ext}}-\tau_{\mathrm{sc}}^h-\tau_b^h+\tau_f^h+\tau_a^h-\tau_p^h)] = 0. \tag{A12}$$

This result can be checked by simple substitution.

In the absence of external stress ($\tau_{\mathrm{ext}}=0$), the general Eqs. (A10)–(A12) can be simplified because for symmetry reasons $d^{+-}(\boldsymbol{r},t)=d^{-+}(\boldsymbol{r},t)$ for every t. In other words, at zero external stress, if one alters the sign of all dislocations, it does not affect the behavior of the system. This means that $d_a=0$ and so, $\tau_f^h=\tau_p^h=0$. In this case, the resulting evolution equations are

$$\partial_t d^{++} + 2\,\nabla\,[\boldsymbol{b}(1+d^{++})(\tau_{\text{ind}}+\tau_{\text{sc}}^h+\tau_b^h+\tau_a^h)]=0, \tag{A13}$$

$$\partial_t d^{+-} + 2\,\nabla\,[\boldsymbol{b}(1+d^{+-})(-\tau_{\text{ind}}-\tau_{\text{sc}}^h-\tau_b^h+\tau_a^h)]=0. \tag{A14}$$

*ispanovity@metal.elte.hu
†groma@metal.elte.hu
‡gyorgyi@glu.elte.hu

[1] D. Walgraef and E. C. Aifantis, J. Appl. Phys. **58**, 688 (1985).
[2] D. Walgraef and E. C. Aifantis, Int. J. Eng. Sci. **23**, 1359 (1985).
[3] J. Kratochvíl and S. Libovický, Scr. Metall. **20**, 1625 (1986).
[4] J. Kratochvíl and M. Saxlová, Scr. Metall. Mater. **26**, 113 (1992).
[5] I. Groma, Phys. Rev. B **56**, 5807 (1997).
[6] I. Groma and P. Balogh, Acta Mater. **47**, 3647 (1999).
[7] M. Zaiser, M. Carmen Miguel, and I. Groma, Phys. Rev. B **64**, 224102 (2001).
[8] I. Groma, F. F. Csikor, and M. Zaiser, Acta Mater. **51**, 1271 (2003).
[9] S. Yefimov, I. Groma, and E. Van der Giessen, J. Mech. Phys. Solids **52**, 279 (2004).
[10] S. Yefimov, I. Groma, and E. Van der Giessen, Modell. Simul. Mater. Sci. Eng. **12**, 1069 (2004).
[11] A. El–Azab, Phys. Rev. B **61**, 11956 (2000).
[12] A. El–Azab, J. Deng, and M. Tang, Philos. Mag. **87**, 1201 (2007).
[13] J. Deng and A. El–Azab, J. Comput.-Aided Mater. Des. **14**, 295 (2007).
[14] F. F. Csikor, I. Groma, T. Hochrainer, D. Weygand, and M. Zaiser, in Proceedings of the 11th International Symposium on Continuum Models and Discrete Systems, edited by D. Jeulin and S. Forest (Mines ParisTech Les Presses, Paris, 2007), p. 271.
[15] M. Zaiser and T. Hochrainer, Scr. Mater. **54**, 717 (2006).
[16] T. Hochrainer, M. Zaiser, and P. Gumbsch, Philos. Mag. **87**, 1261 (2007).
[17] M. Zaiser, N. Nikitas, T. Hochrainer, and E. C. Aifantis, Philos. Mag. **87**, 1283 (2007).
[18] C. Schwarz, R. Sedláček, and E. Werner, Acta Mater. **56**, 341 (2008).
[19] R. Sedláček, J. Kratochvíl, and E. Werner, Philos. Mag. **83**, 3735 (2003).
[20] I. Groma, G. Györgyi, and B. Kocsis, Phys. Rev. Lett. **96**, 165503 (2006).
[21] I. Groma, G. Györgyi, and B. Kocsis, Philos. Mag. **87**, 1185 (2007).
[22] V. Vinogradov and J. R. Willis, Int. J. Solids Struct. **45**, 3726 (2008).
[23] V. Vinogradov and J. R. Willis (unpublished).
[24] J. G. Kirkwood, J. Chem. Phys. **3**, 300 (1935).
[25] R. Balescu, *Equilibrium and Nonequilibrium Statistical Mechanics* (Wiley, New York, 1975), p. 245.
[26] M. Wilkens, Acta Metall. **17**, 1155 (1969).