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Kinetic theory of dislocations: a time-dependent projection-operator approach

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In this paper we develop a kinetic theory for interacting dislocation systems. Dislocations interact via a long range $1/r$-type force so that the system will be spatially inhomogeneous. A new kinetic equation is obtained using the time-dependent projection operator formalism of Willis and Picard. An exact equation for the time evolution of the one-particle probability density is obtained, which can be approximated as a closed Markovian equation in the approximation that the time scale of fluctuations is much shorter than the relaxation and dynamical time scales. The core of the distribution of dislocation velocity fluctuations is found to be Gaussian, while the high-velocity tail decays algebraically. A well-defined non-vanishing self-consistent mean field can be isolated for which we recover precisely the same expression as Groma obtained by a truncation of the BBGKY hierarchy of dislocation distribution functions.

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1. Introduction

It is well known that during plastic flow of crystalline materials dislocations, the carriers of plastic deformation tend to form nonuniform, highly organized structures. Several analytical models (the concept of Low Energy Dislocation Structure proposed by Kulhman-Wilsdorf [1], the models of Holt [2] and Rickman & Viñals [3] that apply irreversible thermodynamics analogy, the reaction-diffusion approach elaborated by Walgraef and Aifantis [4], the concept of the dislocation sweeping mechanism developed by Kratochvil et. al. [5], and the Ananthakrishna model [6, 7] of coupled nonlinear rate equations for the dislocation densities have been developed since dislocation patterning was first observed.

Due to limitation of continuum models to account for the details of the underlying physical mechanisms governing dislocation motion and interactions, discrete dislocation simulations have been proposed as an alternative to continuum phenomenological approaches mentioned above (see e.g. [8, 9] for a review of various continuum and discrete dislocation simulation methods proposed to address the problem of dislocation patterning).

An alternative method which was developed as a compromise between discrete dislocation dynamics arguments and continuum approaches for modeling the evolution of dislocation populations at the mesoscale is the so called stochastic approach [10, 11, 12, 13].

A self-consistent mean field approach for dislocation interactions was developed by Groma [14] starting from an equilibrium BBGKY-like hierarchy of dislocation distribution functions corresponding to the Kirkwood approximation in the plasma physics. Later these continuum equations were developed further [15], introducing new gradient terms, by taking into account also the two-body distribution functions.

The use of projection operator techniques developed by Willis and Picard [16] for coupled quantum mechanical density matrices has become increasingly common. This technique was successfully used for classical nonideal gas interacting through two-body forces and for quantum optics [16], two-dimensional turbulence [17, 18], and self-graviting systems [19].

The projection operator techniques which are standard in statistical mechanics are applied here to a system of interacting dislocations. We are interested here in the relaxation of an initially uncorrelated system towards the equilibrium. We chose at random a reference dislocation driven in the first approximation by the smooth self-consistent mean-field velocity induced by a ,,sea of field dislocations" and rapid fluctuations arising from the departure to the mean field. The starting point of our analysis is the Liouville equation for the N-particle distribution function in the phase space. Since our system consist in a large number of dislocations, such an analysis provides much more information one can actually interpret. Consequently we would like to describe the system in some well-defined average sense by introducing differential equations for the time evolution of the one-particle probability density in a one-particle phase space.

In the next sections we revisit the dislocation motion in the crystals and the projection operator formalism. Then we apply this formalism to our dislocation system, deriving an exact equation for the time evolution of the one-particle probability density. In this context the dislocation velocity fluctuations in a nearly homogeneous, parallel, straight edge dislocation system is studied. It is shown that the distribution function has a Gaussian core and an algebraic tail. A well-defined non-vanishing self-consistent mean velocity field is also isolated for which we recover precisely the same expression as Groma obtained [14] by a truncation of the BBGKY hierarchy of dislocation distribution functions.

2. Dislocation motion in the crystals

Dislocation motion in the glide plane is in the direction of Burgers vector for edge dislocations and orthogonal to the Burgers vector for screw dislocations. Screw dislocations can also cross slip between glide planes. The motion of a dislocation perpendicular to the glide plane is called climb.

Due to the long-range nature of interaction forces the internal force acting on a reference dislocation is the sum of forces created by all the other dislocations of the system. The force from a test dislocation j acting on the reference dislocation i is given by the Peach-Koehler equation:

$$\mathbf{F}_{ji} = (\mathbf{b}_i \sigma^j_{\text{int}}) \times \mathbf{l}_i, \tag{2.1}$$

where $\mathbf{b}_i$ is the Burgers vector and $\mathbf{l}_i$ represents the sense vector of the reference dislocation. If the test dislocation is in different slip geometry, the stress tensor σ_{int} is determined by transforming the stress tensor σ of the test dislocation into the reference coordinate system. The total stress tensor acting on the reference dislocation can be computed by summing up contributions from all dislocations in the system.

It is widely accepted that if the crystal has a large Peierls barrier, the inertial forces arising from the dislocation's acceleration are negligible compared to the drag forces, which are taken to be proportional to the dislocation velocity. Then the glide and climb velocity of i^{th} dislocation can be given by

$$\mathbf{v}^i_g = \Gamma_g \mathbf{F}^i_g, \qquad \text{and} \tag{2.2}$$
$$\mathbf{v}^i_c = \Gamma_c \mathbf{F}^i_c. \tag{2.3}$$

where F^i_g and F^i_c is the net force in the glide and climb directions (the sum of Peach-Koehler force projections produced by all the other dislocations to the glide and climb direction) and $\Gamma_{g,c}$ represents the mobilities in the glide and climb directions.

3. The projection operator formalism

Let us consider a collection of $N+1$ parallel straight edge or $N+1$ screw dislocations positioned at the points $\mathbf{r}_i$, $i = \overline{0,N}$ in the xy plane perpendicular to the dislocation lines. We select one of these dislocations, for example dislocation 0 and call it the reference dislocation. The other dislocations $\overline{1,N}$ will be referred as field dislocations. The correct starting point for the analysis of the dynamics of our dislocation system is presumably the Liouville equation for the $N+1$-particle distribution function $\mu(\mathbf{r}, \mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N, t)$ of the system

$$\frac{\partial \mu}{\partial t} + \sum_{i=0}^{N} \frac{\partial}{\partial \mathbf{r}_i}(\mu \mathbf{v}^i) = 0, \tag{3.1}$$

where $\mathbf{v}^i = \mathbf{v}^i_g + \mathbf{v}^i_c$ is the velocity of i^{th} dislocation according to Eqs. (2.2) and (2.3).

If the reference dislocation is described by the variable $x \equiv \mathbf{r}$, and the N-dislocation field by the variable $y \equiv (\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N)$, then we can define, following the original notations of Kandrup [19], the one- and N-particle distribution functions $f(x,t)$ and $g(y,t)$ as

$$f(x,t) = \int dy \mu(x,y,t), \tag{3.2}$$

$$g(y,t) = \int dx \mu(x,y,t). \tag{3.3}$$

The composite distribution function μ can be written in the form

$$\mu(x,y,t) = f(x,t)g(y,t) + \mu_I(x,y,t). \tag{3.4}$$

If our system initially is completely uncorrelated, then the mathematically well-defined problem is to obtain the solutions $f(x,t)$ and $g(y,t)$ subject to the initial conditions

$$\mu_I(x,y,0) = 0, \tag{3.5}$$

$$g(y,0) = \prod_{i=1}^{N} f(y_i,0). \tag{3.6}$$

The Liouville equation (3.1) can be written formally as

$$\frac{\partial \mu(x,y,t)}{\partial t} = -iL\mu = -i(L_0 + L_{\text{sys}} + L_I)\mu, \tag{3.7}$$

where the operators L_0 and L_{sys} act respectively only on the variables x and y, whereas the interaction Liouvillian L_I acts upon both x and y. One can define a new function, supposedly „relevant" function, as

$$\mu_R(x,y,t) = f(x,t)g(y,t). \tag{3.8}$$

In order to obtain decoupled equations for μ_R and μ_I we introduce the time-dependent projection [19, 16]

$$P(x,y,t) = g(y,t) \int dy + f(x,t) \int dx - f(x,t)g(y,t) \int dx \int dy \tag{3.9}$$

with the property that

$$P(x,y,t)\mu(x,y,t) = \mu_R(x,y,t), \quad \text{and} \tag{3.10}$$

$$[1 - P(x,y,t)]\,\mu(x,y,t) = \mu_I(x,y,t). \tag{3.11}$$

One verifies that $P^2(x,y,t) = P(x,y,t)$. Applying P and $1-P$ on the Liouville equation (3.7) we directly obtain the coupled equations

$$\frac{\partial \mu_R}{\partial t} = -iPL\mu_R - iPL\mu_I \tag{3.12}$$

$$\frac{\partial \mu_I}{\partial t} = -i(1-P)L\mu_R - i(1-P)L\mu_I. \tag{3.13}$$

By introducing the Greenian $\mathscr{G}(t,t')$ defined as [16]

$$\mathscr{G}(t,t') = \mathscr{T} \exp\left\{-i\int_{t'}^{t} dt''[1-P(t'')]L\right\}, \tag{3.14}$$

where $\mathscr{T}$ is the Dyson time-ordering operator, we can write down the formal solution of Eq. (3.13) as [19]

$$\mu_I(x,y,t) = \mathscr{G}(t,0)\mu_I(x,y,0) - \int_0^t dt'\mathscr{G}(t,t')[1-P]L\mu_R(x,y,t). \tag{3.15}$$

For an initially uncorrelated system $\mu_I(t=0) \equiv 0$. Having this in mind from Eq. (3.12) one gets

$$\frac{\partial \mu_R}{\partial t} = -iPL\mu_R - \int_0^t dt' PL\mathscr{G}(t,t')[1-P]L\mu_R(x,y,t'). \tag{3.16}$$

By integrating this equation over the variables x and y one gets [19]

$$\frac{\partial f}{\partial t} + iL_0 f + i\langle L_I\rangle_{\text{sys}} f = \int_0^t dt' \int dy \Delta_t L_I \mathscr{G}(t,t')\Delta_{t'} L_I g(y,t') f(x,t') \tag{3.17}$$

and

$$\frac{\partial g}{\partial t} + iL_{\text{sys}} g - i\langle L_I\rangle' g = -\int_0^t dt' \int dx \Delta_t L_I \mathscr{G}(t,t')\Delta_{t'} L_I g(y,t') f(x,t'), \tag{3.18}$$

where the abbreviations

$$\langle L_I\rangle_{\text{sys}} = \int dy' L_I(x,y') g(y',t), \tag{3.19}$$

$$\langle L_I\rangle' = \int dx' L_I(x',y) f(x',t), \tag{3.20}$$

$$\Delta_t L_I = L_I - \langle L_I\rangle_{\text{sys}} - \langle L_I\rangle' \tag{3.21}$$

were introduced.

4. Derivation of the kinetic equations

The Liouville equation (3.1) can be rewritten as

$$\frac{\partial \mu}{\partial t} + \sum_{i=1}^{N}\left[\frac{\partial}{\partial \mathbf{r}}(\mu \mathbf{v}_{i0}) + \frac{\partial}{\partial \mathbf{r}_i}(\mu \mathbf{v}_{0i})\right] + \sum_{i=1}^{N}\sum_{\substack{j=1\\ j\neq i}}^{N} \frac{\partial}{\partial \mathbf{r}_i}(\mu \mathbf{v}_{ji}) = 0, \tag{4.1}$$

where $\mathbf{v}_{ij}$ denotes the velocity created by dislocation i on the dislocation j.

From Eq. (4.1) one can identify the different operators appearing in the decomposition (3.7):

$$\begin{aligned} iL_0\mu &= 0, \\ iL_{\text{sys}}\mu &= \sum_{i=1}^{N}\sum_{\substack{j=1\\ j\neq i}}^{N} \frac{\partial}{\partial \mathbf{r}_i}(\mu \mathbf{v}_{ji}), \\ iL_I\mu &= \sum_{i=1}^{N}\left[\frac{\partial}{\partial \mathbf{r}}(\mu \mathbf{v}_{i0}) + \frac{\partial}{\partial \mathbf{r}_i}(\mu \mathbf{v}_{0i})\right]. \end{aligned} \tag{4.2}$$

The mean-field velocity created by the field dislocation i on the reference dislocation can be computed as

$$\langle \mathbf{v}_{i0} \rangle = \int f(\mathbf{r}_i, t)\, \mathbf{v}_{i0}\, d\mathbf{r}_i. \tag{4.3}$$

The total mean-field velocity experienced by the reference dislocation is given by the sum of all contributions of the field dislocations

$$\mathbf{v}_{\mathrm{sc}} = \sum_{i=1}^{N} \langle \mathbf{v}_{i0} \rangle = \sum_{i=1}^{N} \langle \mathbf{v}_{10} \rangle = N \langle \mathbf{v}_{10} \rangle. \tag{4.4}$$

By introducing the dislocation density functions $\rho(\mathbf{r},t) = N f(\mathbf{r},t)$ and taking into account Eqs. (2.2) and (2.3) one recovers the same expression for the self-consistent stress as Groma obtained by the truncation of the BBGKY hierarchy of dislocation distribution functions [14]. However, the projection operator approach has the advantage over the standard BBGKY approach because does not require us to introduce a hierarchy of two- and more dislocation distribution functions.

After straightforward integrations by part, one verifies that

$$i\langle L_I \rangle_{\mathrm{sys}} f \;=\; \left[\int dy' g(y',t) \sum_{i=1}^{N} \mathbf{v}_{i0}\right] \frac{\partial f}{\partial \mathbf{r}} + f \left[\int dy' g(y',t) \sum_{i=1}^{N} \frac{\partial \mathbf{v}_{i0}}{\partial \mathbf{r}}\right] = \frac{\partial}{\partial \mathbf{r}}(f \mathbf{v}_{\mathrm{sc}}), \qquad \text{and} \tag{4.5}$$

$$i\Delta_t L_I f \;=\; \sum_{i=1}^{N} \frac{\partial}{\partial \mathbf{r}} \{ f[\mathbf{v}_{i0} - \langle \mathbf{v}_{i0} \rangle] \} + \sum_{i=1}^{N} \frac{\partial}{\partial \mathbf{r}_i} \{ f[\mathbf{v}_{0i} - \langle \mathbf{v}_{0i} \rangle] \}. \tag{4.6}$$

Using that $\mathbf{v}_{i0} = -\mathbf{v}_{0i}$, we define the fluctuating velocity $\mathscr{V}_{0i}(\mathbf{r}, \mathbf{r}_i, t)$ that the i^{th} field dislocation at $\mathbf{r}_i$ exerts upon the reference dislocation at $\mathbf{r}$ as

$$\mathscr{V}_{0i}(\mathbf{r}, \mathbf{r}_i, t) = \mathrm{v}_{0i}(\mathbf{r}, \mathbf{r}_i, t) - \mathbf{v}_{\mathrm{sc}}(\mathbf{r}, t), \tag{4.7}$$

and the fluctuation velocity that the reference dislocation exerts upon the i^{th} field dislocation at $\mathbf{r}_i$ as

$$\mathscr{V}_{i0}(\mathbf{r}, \mathbf{r}_i, t) = -\mathrm{v}_{0i}(\mathbf{r}, \mathbf{r}_i, t) - \mathbf{v}_{\mathrm{sc}}(\mathbf{r}_i, t). \tag{4.8}$$

Now we can rewrite our expression for the operator $i\Delta_t L_I$ in the form

$$i\Delta_t L_I \;=\; \sum_{i=1}^{N} \left[\frac{\partial \mathscr{V}_{i0}}{\partial \mathbf{r}} + \mathscr{V}_{i0} \frac{\partial}{\partial \mathbf{r}} \right] + \sum_{i=1}^{N} \left[\frac{\partial \mathscr{V}_{0i}}{\partial \mathbf{r}_i} + \mathscr{V}_{0i} \frac{\partial}{\partial \mathbf{r}_i} \right]. \tag{4.9}$$

In terms of the fluctuating velocities one has then the equation of motion

$$\begin{aligned} \frac{\partial f}{\partial t} + \frac{\partial}{\partial \mathbf{r}}(f \mathbf{v}_{\mathrm{sc}}) = S[f] = \int dy \int_0^t dt' \sum_{i=1}^{N} \left[\frac{\partial \mathscr{V}_{i0}}{\partial \mathbf{r}} + \frac{\partial \mathscr{V}_{0i}}{\partial \mathbf{r}_i} + \mathscr{V}_{i0} \frac{\partial}{\partial \mathbf{r}} + \mathscr{V}_{0i} \frac{\partial}{\partial \mathbf{r}_i} \right] \times \\ \mathscr{G}(t,t') \left\{ \sum_{j=1}^{N} \left[\frac{\partial}{\partial \mathbf{r}} \{ \mathscr{V}_{j0} g(y,t') f(\mathbf{r},t') \} + \frac{\partial}{\partial \mathbf{r}_j} \{ \mathscr{V}_{0j} g(y,t') f(\mathbf{r},t') \} \right] \right\}. \end{aligned} \tag{4.10}$$

The functional $S[f]$ in fact represents the influence of correlations upon the dynamics of the system.

The equation (4.10) is an exact differential equation for $f(x,t)$ subject to the initial condition $\mu_I(x,y,0) = 0$. However, this equation is not directly soluble, since the other unknown function $g(y,t)$ is given by an equation of the form (3.18) depending in turn on $f(x,t)$. The coupled system of equations bears the same information as the initial Liouville equation and without further simplification is untractable.

5. Weakly correlated dislocation systems

5.1 Statistics of velocity fluctuations

An initially decorrelated dislocation system with $\mu_I(x,y,0) = 0$ for sufficiently short times remains decorrelated. Because of the assumed symmetry of μ under dislocation interchange, the choice of the reference dislocation is arbitrary. Since $\mu_I(x,y,0)$ vanishes, in addition we must demand that

$$\mu_R(x,y,0) = f(x,0)\prod_{i=1}^{N} f(\mathbf{r}_i,0). \tag{5.1}$$

We might assume that correlations among the field dislocations will not strongly affect the reference dislocation (which will not be in general true) and expect that such an assumption would be reasonable for time periods δt short compared with the time scale for development of strong correlations. Then, for such time scales the distribution function

$$f(x,t-\delta t)\prod_{i=1}^{N} f(\mathbf{r}_i,t-\delta t) \tag{5.2}$$

can be evaluated at time t and the details of the dynamics and interaction among dislocations during such very short relative times τ can be encapsulated in the Greenian $\overline{\mathscr{G}}(t,t-\delta t)$.

For the sake of simplicity let us consider that our system is a collection of N straight, parallel edge dislocations with Burgers vector $\mathbf{b}$ oriented parallel to the x axis and the dislocation line parallel to the z axis, randomly distributed and confined within a disk of radius R. Furthermore we assume that the dislocations have the same Burgers vector b. We are particularly interested in the ,,thermodynamic limit" in which the number of dislocations and the size of the domain go to infinity ($N \to \infty$, $R \to \infty$) in such a way that the dislocation density $\rho = \frac{N}{\pi R^2}$ remains finite.

If the temperature is low, the dislocation climb can be neglected and the equation of motion of i^{th} dislocation (2.2) reduces to

$$\mathbf{v_i} \equiv \frac{d\mathbf{r}_i}{dt} = \Gamma_g \mathbf{b_i} \sum_{j\neq i} \tau_{\text{ind}}^{j}(x_j - x_i, y_j - y_i), \qquad j = \overline{1,N} \tag{5.3}$$

where $\mathbf{r_i} \equiv (x_i, y_i)$ denotes the position of the i-th dislocation and

$$\tau_{\text{ind}}^{i}(x,y) = \frac{\mu b_i}{2\pi(1-\nu)} \frac{x(x^2-y^2)}{(x^2+y^2)^2} \equiv \phi_i \tag{5.4}$$

is the shear stress created by an edge dislocation (in an infinite domain), where the shear modulus μ and the Poisson's ratio ν were introduced. Since the dislocations are randomly distributed, the stress τ fluctuates.

The first problem to consider is the characterization of the velocity fluctuations. The velocity in Eq. (5.3) is proportional to the shear stress, therefore finding the velocity distribution is equivalent with finding the stress distribution function at a point where the dislocation is located.

The stress distribution $P_N(\tau)$ in a system of N uncorrelated, identical dislocation system can be obtained as a direct application of Markov's method [20] applied for several problems. As it was shown by Groma and Bakó [11], the internal stress distribution can be expressed as

$$P_N(\tau) = \int \prod_{i=1}^{N} \rho_d(\mathbf{r}_i) d\mathbf{r}_i \delta(\tau - \sum_{i=1}^{N} \phi_i) \tag{5.5}$$

where $\rho_d(\mathbf{r}_i)d\mathbf{r}_i$ governs the probability of occurrence of the i^{th} dislocation at position $\mathbf{r}_i$. Using the Markov's method, we can express $\delta(x)$ in terms of its Fourier transform

$$\delta(x) = \frac{1}{2\pi} \int \exp(-iqx) dq. \tag{5.6}$$

Then $P_N(\tau)$ becomes

$$P_N(\tau) = \frac{1}{2\pi} \int A_N(q) \exp(-iq\phi) dq. \tag{5.7}$$

with

$$A_N(q) = \left[\int_{|\mathbf{r}|=0}^{R} \exp(iq\phi) \rho_d(\mathbf{r}) d\mathbf{r} \right]^N. \tag{5.8}$$

If we suppose that the dislocations are uniformly distributed on average, then $\rho_d(\mathbf{r}) = \pi^{-1} R^{-2}$ and

$$A_N(q) = \left[\frac{1}{\pi R^2} \int_{|\mathbf{r}|=0}^{R} \exp(iq\phi) d\mathbf{r} \right]^N = \left[1 - \frac{1}{\pi R^2} \int_{|\mathbf{r}|=0}^{R} [1 - \exp(iq\phi)] d\mathbf{r} \right]^N \tag{5.9}$$

In the limit when $N \to \infty$ and $R \to \infty$ in such way that the density $\rho = N/(\pi R^2)$ remains finite, if the integral in (5.9) increases less rapidly than N, then the limiting process $A(q) = \exp[-\rho C(q)]$ where

$$C(q) = \int_{|\mathbf{r}|=0}^{R} [1 - \exp(iq\phi)] d\mathbf{r} = \int_0^R \int_0^{2\pi} \left[1 - \cos\left(qGb \frac{\cos(\theta)\cos(2\theta)}{r} \right) \right] r dr d\theta, \tag{5.10}$$

with $G = \dfrac{\mu}{2\pi(1-\nu)}$, is permissible.

For small arguments $\cos(x) = 1 - x^2/2 + \mathscr{O}(x^4)$ and we obtain

$$C(q) \approx \frac{\pi}{8} G^2 b^2 q^2 \ln \left[\frac{N}{\pi \rho G^2 b^2 q^2} \right]. \tag{5.11}$$

Since $C(q)$ diverges weakly (logarithmically) with N, we have the estimate

$$A(q) = \exp \left[-\frac{\pi}{8} G^2 b^2 \rho q^2 \ln \left(\frac{N}{\pi \rho G^2 b^2 q^2} \right) \right]. \tag{5.12}$$

When $N \to \infty$,

$$A(q) = \exp \left[-q^2 \frac{\pi}{8} G^2 b^2 \rho \ln N \right], \tag{5.13}$$

and for $q \to 0$ we obtain

$$A(q) = \exp \left[\frac{\pi}{4} G^2 b^2 \rho q^2 \ln |q| \right], \tag{5.14}$$

The stress distribution $P(\tau)$ is simply the Fourier transform of $A(q)$.

The core of the stress distribution function can be determined taking into account that for small stresses the integral in Eq. (5.7) is negligible and we can use $A(q)$ given by Eq. (5.13). Then the distribution $P(\tau)$ is the Gaussian

$$P(\tau) = \sqrt{\frac{2}{\pi^2 G^2 b^2 \rho \ln N}} \exp\left[-\frac{2\tau^2}{\pi G^2 b^2 \rho \ln N}\right] \tag{5.15}$$

The high stress tail of the distribution can be calculated from Eq. (5.14). This problem was studied by Groma and Bakó [11] and was found that the tail of the distribution function decays algebraically like τ^{-3}:

$$P(\tau) = \frac{\pi G^2 b^2 \rho(\mathbf{r})}{4\tau^3} \tag{5.16}$$

For a nearly homogeneous dislocation system Eq. (5.9) has the form

$$A_N(q) = \left[\int_{|\mathbf{r}|=0}^{R} f(\mathbf{r}) \exp(iq\phi) d\mathbf{r}\right]^N = \left[1 - \frac{1}{N}\int_{|\mathbf{r}|=0}^{R} \rho(\mathbf{r})[1-\exp(iq\phi)]d\mathbf{r}\right]^N \tag{5.17}$$

Repeating the previous steps and taking into the account the relation between the velocity and stress given by Eq. (5.3), one finds that the core of the velocity distribution function is Gaussian,

$$P(\mathcal{V}) = \sqrt{\frac{2}{\pi^2 G^2 \Gamma_g^2 b^2 \rho(\mathbf{r}) \ln N}} \exp\left[-\frac{2\mathcal{V}^2}{\pi G^2 \Gamma_g^2 b^2 \rho(\mathbf{r}) \ln N}\right], \tag{5.18}$$

and for large values of $\mathcal{V}$ the velocity distribution decays algebraically:

$$P(\mathcal{V}) = \frac{\pi G^2 \Gamma_g^2 b^2 \rho(\mathbf{r})}{4\mathcal{V}^3}, \tag{5.19}$$

where $\mathcal{V} = v - \langle v \rangle$ is the velocity fluctuation around the local mean-field velocity given by Eq. (4.4). The approximations used here are valid as long the factorization hypothesis given by Eq. (5.1) is valid. In the strict mathematical limit $N \rightarrow \infty$ the transition between the two regimes given by Eqs. (5.18) and (5.19) is rejected to infinity and $P(v)$ is purely Gaussian. However, the convergence towards the Gaussian distribution is very slow and in practice we will always see the algebraic tail in computer simulations.

The previous results are valid if the velocity fluctuations are calculated at a fixed point. In this case it is no restriction on the possible values of the stress. However, if we are interested in the stress experienced by the reference dislocation, the situation is different, since a dipole can form when a field dislocation approaches the reference dislocation and our treatment which ignores the correlations between the dislocations will break down.

The distribution of stresses in a system of dislocation dipoles was studied by Csikor and Groma [21]. It was found that the core of the stress distribution function becomes Lorentzian, but the high-stress tail of the distribution has an algebraic decay given by Eq. (5.16). That means that the high velocity tail of the distribution $P(\mathcal{V})$ remains still valid for a gas of dislocation dipoles.

5.2 The kinetic equation

If we assume, that the trajectories of the dislocations between $t-\delta t$ are determined by the complicated Greenian $\overline{\mathscr{G}}(t,t-\delta t)$, for sufficiently short times δt, the approximation (5.2) introduced in Eq. (4.10) leads to

$$\frac{\partial f}{\partial t}+\frac{\partial}{\partial \mathbf{r}}(f\mathbf{v}_{\rm sc})=\int dy\int_0^t d\tau\sum_{i=1}^N\left[\frac{\partial \mathscr{V}_{i0}}{\partial \mathbf{r}}+\frac{\partial \mathscr{V}_{0i}}{\partial \mathbf{r}_i}+\mathscr{V}_{i0}\frac{\partial}{\partial \mathbf{r}}+\mathscr{V}_{0i}\frac{\partial}{\partial \mathbf{r}_i}\right]\overline{\mathscr{G}}(t,t-\tau)\times$$
$$\left\{\sum_{j=1}^N\left[\frac{\partial}{\partial \mathbf{r}}\{\mathscr{V}_{j0}f(\mathbf{r},t-\tau)\prod_{k=1}^N f(\mathbf{r}_k,t-\tau)\}+\frac{\partial}{\partial \mathbf{r}_j}\{\mathscr{V}_{0j}f(\mathbf{r},t-\tau)\prod_{k=1}^N f(\mathbf{r}_k,t-\tau)\}\right]\right\}. \quad (5.20)$$

In this approximation we have obtained a closed nonlinear integro-differential equation for $f(\mathbf{r},t)$ in terms of its past history.

Close to equilibrium, to a good approximation, we can consider that the dislocations are purely advected by the equilibrium mean-field stress, therefore we can replace the exact Greenian with a smooth Greenian $\langle\mathscr{G}\rangle_{\rm eq}$ constructed formally with the averaged Liouville operator, since the fluctuation $\mathscr{V}$ for $N\to\infty$ is much smaller, than the equilibrium mean-field velocity $\langle\mathbf{v}\rangle_{\rm eq}$. In this approximation Eq. (5.20) can be simplified considerably:

$$\frac{\partial f}{\partial t}+\frac{\partial}{\partial \mathbf{r}}(f\langle\mathbf{v}\rangle_{\rm eq})=\int dy\int_0^t d\tau\sum_{i=1}^N\left[\mathscr{V}_{i0}\frac{\partial}{\partial \mathbf{r}}+\mathscr{V}_{0i}\frac{\partial}{\partial \mathbf{r}_i}\right]\times$$
$$\langle\mathscr{G}(t,t-\tau)\rangle_{\rm eq}\left\{\sum_{j=1}^N\left[\mathscr{V}_{j0}\frac{\partial}{\partial \mathbf{r}}+\mathscr{V}_{0j}\frac{\partial}{\partial \mathbf{r}_j}\right]\{f(\mathbf{r},t-\tau)\prod_{k=1}^N f_{\rm eq}(\mathbf{r}_k,t-\tau)\}\right\}, \quad (5.21)$$

where $\langle\rangle_{\rm eq}$ represents the average with respect to the equilibrium distribution $f_{\rm eq}(\mathbf{r})$. After an integration by parts over the spatial variables Eq. (5.21) reduces to

$$\frac{\partial f}{\partial t}+\frac{\partial}{\partial \mathbf{r}}(f\langle\mathbf{v}\rangle_{\rm eq})=\frac{\partial}{\partial r^\mu}\int dy\int_0^t d\tau\sum_{i=1}^N\sum_{j=1}^N\mathscr{V}_{i0}^\mu(t)\langle\mathscr{G}(t,t-\tau)\rangle_{\rm eq}\times$$
$$\left[\mathscr{V}_{j0}^\nu(t-\tau)\frac{\partial}{\partial r^\nu}+\mathscr{V}_{0j}^\nu(t-\tau)\frac{\partial}{\partial r_j^\nu}\right]f(\mathbf{r},t-\tau)\prod_{k=1}^N f_{\rm eq}(\mathbf{r}_k) \quad (5.22)$$

This equation resembles a Fokker-Planck equation in which the first term of the right-hand side corresponds to a diffusion and the second term to a drift.

Assuming, that in first approximation the dislocations follow streamlines, after explicating the action of the Greenian, we can rewrite Eq. (5.22) in the form

$$\frac{\partial f}{\partial t}+\frac{\partial}{\partial \mathbf{r}}(f\langle\mathbf{v}\rangle_{\rm eq})=$$
$$\sum_{i=1}^N\frac{\partial}{\partial r^\mu}\int d\mathbf{r}_i\int_0^t d\tau\mathscr{V}_{i0}^\mu(t)\left[\mathscr{V}_{i0}^\nu(t-\tau)\frac{\partial}{\partial r^\nu}+\mathscr{V}_{0i}^\nu(t-\tau)\frac{\partial}{\partial r_i^\nu}\right]f(\mathbf{r},t-\tau)f_{\rm eq}(\mathbf{r}_i) \quad (5.23)$$

Since the field dislocations are identical, we also have

$$\frac{\partial f}{\partial t}+\frac{\partial}{\partial \mathbf{r}}(f\langle\mathbf{v}\rangle_{\rm eq})=$$
$$N\frac{\partial}{\partial r^\mu}\int d\mathbf{r}_1\int_0^t d\tau\mathscr{V}_{10}^\mu(t)\left[\mathscr{V}_{10}^\nu(t-\tau)\frac{\partial}{\partial r^\nu}+\mathscr{V}_{01}^\nu(t-\tau)\frac{\partial}{\partial r_1^\nu}\right]f(\mathbf{r},t-\tau)f_{\rm eq}(\mathbf{r}_1) \quad (5.24)$$

The analytical expression of the velocity fluctuation correlation function and of the equilibrium distribution $f_{\mathrm{eq}}(\mathbf{r}_1)$ need further investigations. Since these functions are not known yet, we cannot transform this integro-differential equation into a Fokker-Planck equation. However, regarding the velocity fluctuations as Markovian random variables, and by making an appropriate guess for the function f_{eq}, we might be able to evaluate the diffusion tensor and the drift term.

6. Conclusion

In this paper, we have provided a systematic derivation of the Landau equation for dislocations, applying the powerful projection operator techniques to this problem. The kinetic equation can be derived by focusing on a reference dislocation and considering its interaction with the remaining ,,field dislocations".

There are different methods to obtain a kinetic equation for the distribution function $f(\mathbf{r},t)$. One possibility is to close the BBGKY hierarchy by neglecting the cumulant of the three-body correlation function [14], [15]. However, the projection operator formalism has the advantage over the standard BBGKY approach that it takes into account non Markovian effects and spatial delocalization.

Some analytical properties of velocity fluctuation distribution function are determined for the idealized case of a system of almost uncorrelated, straight, parallel edge dislocations in single slip configuration. It was shown that the core of the distribution is Gaussian, while the high-velocity tail decays with the third power of the velocity fluctuations. Due to the velocity fluctuations the motion of the dislocations can be regarded as an effective diffusion and drift.

The analytical form of the diffusion cannot be determined for the moment. However, it seems to be influenced by the autocorrelations of the velocity fluctuation. A numerical work in progress by the author shows that the velocity fluctuations have long-term correlations and they are more complex than the usual white noise effect. When memory effects are ignored, we obtain a Fokker-Planck equation of the one-particle distribution function for the system close to equilibrium.

Eq. (5.24) resemble the equations of original Aifantis [22], W–A (Walgraef–Aifantis) [4], and Groma-Zaiser models [23]. The equations studied in this paper correspond to conserved number of dislocations, i.e. they do not describe dislocation creation and annihilation. However, it is easy to lift this strong limitation by adding a source term to the right hand side of Eq. (4.10). Although this is a very important issue, it is out of the scope of the present paper.

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