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LETTER TO THE EDITOR

Mean-field solution of the statistical dislocation pile-up problem by means of a quantum analogy

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Abstract. It is shown that the thermal equilibrium distribution of pile-up dislocations in a stressed crystal can be obtained by solving self-consistently a mean-field single-particle Schrödinger equation. This last equation is derived exactly, using a variational technique, from a many-particle Schrödinger equation formerly shown to be equivalent to a multivariate Fokker–Planck equation for the dislocation positions' joint probability density. Hinging on the proved existence and uniqueness of the solution, a uniformly converging iterative procedure has been built and used to find numerically the pile-up density and mean field. Analogies (and differences) between this problem and the iterative solution of Hartree's equations for many-electron atoms are outlined.

There are several problems in classical statistical physics which can be modelled by means of generalized Langevin equations. In the case of the well known dislocation pile-up model (see e.g. [1] and references therein) the presence of both random forces (to simulate thermal agitation near thermodynamic equilibrium) and dissipative forces was treated for the first time by one of us [2] in the frame of the associated Fokker–Planck equation [14]. The model describes a population of straight, parallel, infinite dislocations of either screw or edge character gliding on a crystal plane under the action of both internal and external forces. In this way the dislocation–dislocation, dislocation–phonon and dislocation–other defects interactions can be accounted for in a statistical treatment using the fluctuation–dissipation theorem. Complex real world effects, such as configurational entropy contributions related to the curvature of dislocation lines (loops and networks) were not taken into account. This has a twofold justification. Firstly there are several physical situations where those effects can be neglected [1], as it has been known for many years. Secondly, if considered, the resulting field equations can only be contemplated with a hopeless frustration [3].

In a successive paper it was shown [4] that the density and the mean field of a linear dislocation pile-up in a stressed crystal in thermodynamic equilibrium can be obtained, at least in principle, by solving the many-body Schrödinger equation:

$$\mathcal{H}\psi_n(\boldsymbol{x}) = \lambda_n \psi_n(\boldsymbol{x}) \tag{1}$$

for the ground state eigenfunction. In (1) the vector $\boldsymbol{x} = [x_i]$ represents the dislocation positions. $\psi(\boldsymbol{x})$ is the joint probability density for $\boldsymbol{x}$, for which a normalization condition holds (we neglect dislocation reactions):

$$\int |\psi(\boldsymbol{x})|^2 \mathrm{d}^N \boldsymbol{x} = 1.$$

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In all equations the dimensionless variables already used in [4] have been used and integrals are between $-\infty$ and $+\infty$.

$$\mathcal{H} = -\mathcal{D}\sum_{i=1}^{N}\frac{\partial^2}{\partial x_i^2} + \mathcal{U}(x_1, ..., x_N) \tag{2}$$

$\mathcal{U}$ being an effective potential energy operator given by

$$\mathcal{U}(x_1, ..., x_N) = \frac{1}{4\mathcal{D}}\sum_{i=1}^{N}\left(\frac{\partial \mathcal{V}}{\partial x_i}\right)^2 - \frac{1}{2}\sum_{i=1}^{N}\frac{\partial^2 \mathcal{V}}{\partial x_i^2}. \tag{3}$$

$\mathcal{H}$ is composed of two parts: (a) a sum of single-particle Hamiltonians $\mathcal{H}_0(x_i)$ plus (b) an interaction operator $\mathcal{H}_p(x)$ which, in general, is not simply a sum of two-body interactions $\mathcal{H}_{2b}$ but contains also three-particle correlations $\mathcal{H}_{3b}$ and interactions between particles and the external field $\mathcal{H}_{fp}$ because of the non-linear terms in (3):

$$\mathcal{H} = \sum_{i=1}^{N}\mathcal{H}_0(x_i) + \mathcal{H}_p \tag{4}$$

$$\mathcal{H}_p = \mathcal{H}_{2b} + \mathcal{H}_{3b} + \mathcal{H}_{fp} \tag{5}$$

$$\mathcal{H}_0(x_i) = -\mathcal{D}\frac{\partial^2}{\partial x_i^2} + \frac{1}{4\mathcal{D}}S^2(x_i) + \frac{1}{2}\frac{\partial S(x_i)}{\partial x_i} \tag{6}$$

$$\mathcal{H}_{2b}(x) = \frac{1}{2}\sum_{i=1}^{N}\sum_{j\neq i}^{1,...,N}\frac{\partial}{\partial x_i}\left[\frac{(2\mathcal{D})^{-1} - 1}{(x_j - x_i)}\right] \tag{7}$$

$$\mathcal{H}_{3b}(x) = \frac{1}{2\mathcal{D}}\sum_{i=1}^{N}\sum_{j\neq i}^{1,...,N}\sum_{k\neq j}^{1,...,N}\frac{1}{(x_j - x_i)(x_j - x_k)} \tag{8}$$

$$\mathcal{H}_{fp}(x) = -\frac{1}{2\mathcal{D}}\sum_{i=1}^{N}S(x_i)\sum_{j\neq i}^{1,...,N}\frac{1}{(x_j - x_i)}. \tag{9}$$

In (1)–(9)

$$\mathcal{D} = \frac{2\pi(1-\nu)K_B T}{\mu b^3}$$

is a dimensionless diffusion coefficient with μ the shear modulus, ν Poisson's ratio†, b the Burgers vector, K_B the Boltzmann constant, and T the absolute temperature.

$$\mathcal{V}(x_1, x_2, \ldots, x_N, t) = \mathcal{V}_{ext} - \frac{1}{2}\sum_{i=1}^{N}\sum_{j\neq i}^{N}\ln|x_i - x_j| \tag{10}$$

is the 'physical' potential energy of the dislocation pile-up in the external field $\mathcal{V}_{ext}$. Well within a crystal grain $\mathcal{V}_{ext} \simeq -x$, as discussed in [4].

In this former paper an approximate procedure, founded only on physical grounds, was used to derive 'single-particle' equations from (1). Here instead we derive and solve an 'exact' single-particle Schrödinger equation using a rigorous variational technique. The form

† This is the case of edge dislocations. The screw case is recovered putting $\nu = 0$.

of the mean-field potential so obtained differs for the presence of three-body interactions (generated by (8)) from standard Hartree-like equations in the quantum mechanics of multielectron atoms. Of course a second fundamental difference resides in the 'boson-like' nature of dislocations in a quasi-linear external field, as shown in [4]. It is also important to note that this is a concrete example where the 'effective quantum mechanics' corresponding to a classical statistical problem can be fully exploited [5, 6], at least as far as the ground state is concerned.

We follow the original Hartree method [8] and seek a product wavefunction:

$$\psi(\boldsymbol{x}) = \prod_{i=1}^{N} \varphi_i(x_i) \tag{11}$$

with

$$\int |\varphi_i(x_i)|^2 \mathrm{d}x_i = 1 \tag{12}$$

describing the 'ground state' of the system. In fact the sole eigenfunction corresponding to minimum eigenvalue ($\lambda_n = 0$) has a physical meaning here, corresponding to thermodynamic equilibrium in the original physical problem [4]. It is known that $\lambda = 0$ is the exact value of λ for the ground state. Equation (11) being an approximate solution, we really look for the minimum possible value of $|\lambda|$ which can never be exactly zero. At this point we make use of the *boson* nature of our *particles* in the external field $-x$, as discussed in [4], and put all *particles* in the same state $\varphi(x_i)$.

Using a standard variational procedure we find the single-particle equation for the wavefunction φ that minimizes the constrained functional

$$\mathcal{B} = \int \left[\mathcal{K}(\varphi, x_i) + \lambda N \varphi^2(x_i)\right] \mathrm{d}x_i \tag{13}$$

where λ is now a Lagrange multiplier and

$$\begin{aligned}\mathcal{K}(\varphi, x_i) = N\Bigg[&\mathcal{D}\left(\frac{\partial \varphi}{\partial x_i}\right)^2 + \varphi^2(x_i)\frac{1}{4\mathcal{D}}S^2(x_i) + \frac{1}{2}\frac{\partial S(x_i)}{\partial x_i}\varphi^2(x_i) \\ &+ \frac{(2\mathcal{D})^{-1} - 1}{2}\varphi^2(x_i)(N-1)\frac{\mathrm{d}}{\mathrm{d}x_i}\left[\int \mathrm{d}x_j \frac{\varphi^2(x_j)}{(x_j - x_i)}\right] \\ &+ \frac{1}{2\mathcal{D}}\varphi^2(x_i)(N-1)(N-2)\int\int \mathrm{d}x_j\,\mathrm{d}x_k \frac{\varphi^2(x_j)\varphi^2(x_k)}{(x_j - x_i)(x_j - x_k)} \\ &- \frac{1}{2\mathcal{D}}\varphi^2(x_i)S(x_i)(N-1)\int \mathrm{d}x_j \frac{\varphi^2(x_j)}{(x_j - x_i)}\Bigg].\end{aligned} \tag{14}$$

All integrals in (14) are meant as Cauchy principal-values ones. The Euler–Lagrange equation takes then the form of a single-particle Schrödinger equation:

$$-\mathcal{D}\mathrm{d}^2\varphi(x_i)/\mathrm{d}x_i^2 + \tilde{U}(x_i)\varphi(x_i) = \lambda\varphi(x_i) \tag{15}$$

where the mean-field potential $\tilde{U}$ is given below.

So far we have reduced a linear many-body equation to the single-particle Schrödinger-like equation (15), where the mean potential $\tilde{U}(x)$ contains two-body, three-body and external field correlation terms:

$$\tilde{U}(x_i) = \frac{1}{4\mathcal{D}}S^2(x_i) + \frac{1}{2}\frac{\partial S(x_i)}{\partial x_i} + \frac{(2\mathcal{D})^{-1}-1}{2}(N-1)\frac{\mathrm{d}}{\mathrm{d}x_i}\left[\int \mathrm{d}x_j \frac{\varphi^2(x_j)}{(x_j - x_i)}\right] + \frac{1}{2\mathcal{D}}(N-1)(N-2)\int \mathrm{d}x_j \frac{\varphi^2(x_j)}{(x_j - x_i)}\int \mathrm{d}x_k \frac{\varphi^2(x_k)}{(x_j - x_k)} - \frac{1}{2\mathcal{D}}S(x_i)(N-1)\int \mathrm{d}x_j \frac{\varphi^2(x_j)}{(x_j - x_i)}. \tag{16}$$

Searching for the ground state of equation (15), which again corresponds to to the minimum value of $|\lambda|$ and to the statistical equilibrium configuration of our system, is very awkward from an analytical point of view. Yet the exact mathematical properties of the solution have been found by one of us and are shown elsewhere [7]. Here, well founded on these results, we have adopted a numerical approach based on a successive approximation method. Equation (15), written in the form

$$\mathcal{D}\mathrm{d}^2\varphi(x)/\mathrm{d}x^2 + \mathcal{Q}(x,\lambda)\varphi(x) = 0 \tag{17}$$

is integrated in a *sufficiently large* finite range by the D02KEF Fortran routine [9] starting with the coefficient

$$\mathcal{Q}_1(x,\lambda) = \lambda - \tilde{U}_0(x) \tag{18}$$

where $\tilde{U}_0$ is simply the shifted harmonic oscillator potential obtained from (16) neglecting all the interaction terms. The routine calculates the normalized ground state eigenfunction $\varphi_{01}(x)$ and the relative eigenvalue λ_{01}. Once φ_{01} is known, the routine D01AQF [9] evaluates all the singular integrals contained in the complete form of the potential in a Cauchy principal-value sense. Therefore we obtain $\tilde{U}_1$ and, immediately

$$\mathcal{Q}_1(x,\lambda) = \lambda_{01} - \tilde{U}_0(x). \tag{19}$$

Repeating the procedure in an iterative way, we construct the sequences of the successive approximations for the minimum eigenvalue $\{\lambda_{0n}\}$, for the ground state eigenfunction $\{\varphi_{0n}\}$, and for the self-consistent potential $\{\tilde{U}_n\}$. It can be shown [7] that these sequences are strongly convergent to a unique limit; therefore our iterative method leads to one and only one ground state solution. Nevertheless, the numerical results reveal that pointwise convergence cannot be obtained in general unless a stabilizing tool is used. We have chosen to iterate the *up-to-date* mean of both the probability density (square of the ground state eigenfunction), and the potential over the values from the first up to the nth step of the procedure. However this trick solves the problem of numerical convergence only in a limited range of N and $\mathcal{D}$ values, when the ratio $N/\mathcal{D}$ is small enough to allow a perturbative approach to equation (15). In fact, in this limit, the mean potential (16) can be considered as a perturbation of a shifted harmonic oscillator potential:

$$\tilde{U}_0(x) = (1/4\mathcal{D})x^2 - \tfrac{1}{2} \tag{20}$$

whose first-order perturbation term is:

$$U^{(1)}(x) = -\frac{1}{2}(N-1)\frac{\mathrm{d}}{\mathrm{d}x}\int \frac{\varphi_0^2(x_j)}{(x_j - x)}\,\mathrm{d}x_j. \tag{21}$$

So, following e.g. [10], we obtain the first-order perturbation of the minimum eigenvalue as:

$$\lambda_0^{(1)} = -N/4\mathcal{D}. \tag{22}$$

The numerical convergence limits can be stated by saying that the method works when it is not too far from being perturbative. In other words we meet a situation analogous to the Debye–Hückel approximation for classical plasmas: thus another physical criterion of convergence could be that the mean potential energy per dislocation [11] must be much less than the mean thermal energy:

$$(\mathrm{d}\overline{U}/\mathrm{d}N) \sim \mu b^3 \ln(l/\langle r\rangle) \sim \mu b^3 \ln(N-1) \ll K_B T \tag{23}$$

where l is the characteristic length of the region where dislocations are located and $\langle r\rangle$ is the mean distance between neighbouring dislocations. In terms of $\mathcal{D}$ we obtain

$$\ln(N-1) \ll \mathcal{D} \tag{24}$$

which is less stringent than $|(22)| \ll 1$ when N is large. To characterize the speed of convergence we need a significant functional of the probability density. We choose the entropy of the distribution defined as:

$$S = -\int \varphi^2(x) \ln(\varphi^2(x))\mathrm{d}x. \tag{25}$$

It is obvious that the ground state solution maximizes entropy, the system being isolated. Keeping $\mathcal{D}$ constant, we noticed that, as N increased, entropy increased too, and the probability density became broader to denote a stronger repulsive interaction among dislocations. Keeping N constant, as $\mathcal{D}$ increased, entropy increased as usual when temperature grows. Furthermore the absolute value of the fundamental eigenvalue was smaller. This proves that, as temperature increases, considering a trial product wavefunction, where all the 'classical particles' are in the same quantum single-particle state, is a good approximation. Figure 1 shows the convergence of the method towards the self-consistent density in a particular case ($\mathcal{D} = 2$ and $N = 9$). For the same values of the parameters figure 2 shows the behaviour of the fundamental eigenvalue as a function of the number of iterations. After a few iterations (about ten) no important changes take place any more either in eigenvalue or in eigenfunction. After 60 iterations the first seven significant figures of the eigenvalue remained unchanged. The entropy trend turned out to be identical.

There exist several methods to solve the purely mechanical dislocation pile-up problem [11]. Only a few authors have dealt with the more complex problem of finding the global thermodynamic equilibrium properties of the pile-up at finite temperature and nobody has computed the density distribution taking fluctuating forces into account [12, 13]. Here, following the suggestion of [4], we have derived, in a rigorous variational way, a Schrödinger-like equation which, once solved, provides the 'single-particle' density of dislocations in thermal equilibrium in an external field. We stress the analogy we have stated between a classical equilibrium statistical mechanics problem and a new effective many-body quantum problem. Also the self-consistent method of solution we used is strictly analogous to the celebrated Hartree method for multielectron atoms, but differs from that in the existence of three-body interactions and in the boson nature of *particles* here involved.

We conclude, pointing out that the method presented above is quite general [14] and not confined to statistical physics of dislocations. In fact the quantum analogy could be taken further and not limited to the self-consistent mean-field approach.

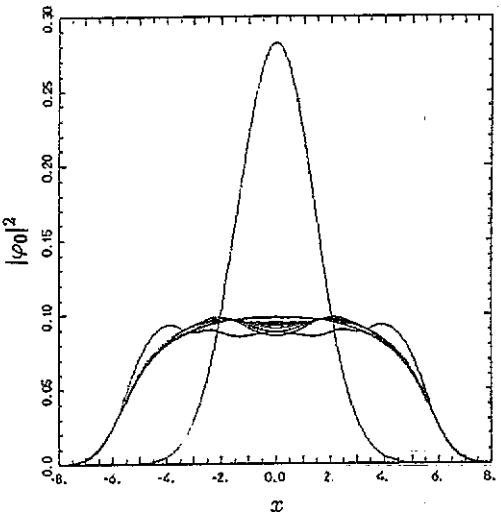

Figure 1. Probability density, square of the ground state eigenfunction $\varphi_0(x)$, versus dislocation position x, as the iterative method proceeds, when $\mathcal{D} = 2$ and $N = 9$. After a few iterations (about ten) substantial convergence is achieved (see text). See also figure 2.

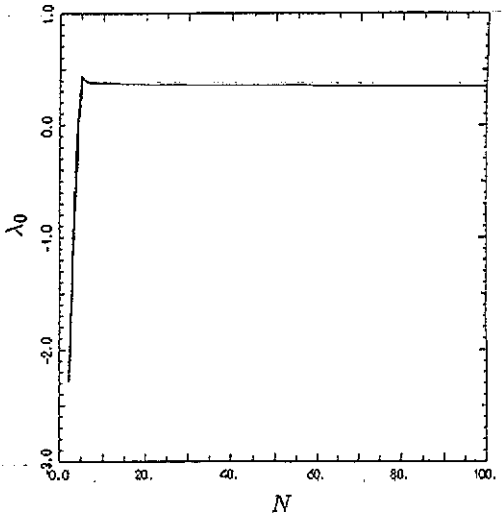

Figure 2. Fundamental eigenvalue versus number of iterations. The numerical values of parameters are the same as in figure 1. The trend of entropy (see text) is quite similar.

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