Analogy between two-dimensional dislocation systems and layered superconductors

J. Cserti

Eötvös University, Department of Physics of Complex Systems, H-1088 Budapest, Múzeum krt. 6-8, Hungary

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We propose a consistent treatment of the applied external stress on a two-dimensional dislocation systems by using the analogy between our model and the layered superconductors. Using the results of a mathematically rigorous, real-space renormalization-group (RG) calculations in the latter model we extend the original model developed by Khantha et al. From our recursion relations a nonlinear equation is derived for the transition temperature as a function of the applied stress. Our results are compared with the predictions of Khantha’s model for three particular materials and the reasons for the deviations are discussed. Possible extensions of our model are outlined.

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In the context of dislocation pattern formation the collective behavior of the dislocation systems seems to play a fundamental role and a new approach has been used to determine the distribution function of the dislocation systems [1]. However, in this model the temperature dependence has not been included. Recently, a new type of mechanism of the cooperative generation of the dislocations has been proposed by Khantha, Pope and Vitek (hereafter referred to as to KPV model) [2]-[3]. The KPV model of the unstable generation of dislocations driven by thermal fluctuation and aided by an applied stress on the solid is based on the theory of the screening of topological defects (vortices) developed by Kosterlitz and Thouless [4] and Berezinskii [5] (hereafter referred as to KTB). The KTB type transition of the topological defects (vortices) has already been well established in several physical systems such as dislocation mediated melting in 2D crystal [6], layered high-temperature superconductors [7], Coulomb gas [8], superfluid 4He films, 2D X-Y model, liquid crystals (for review see [9]).

The KTB phase transition seems to play a fundamental role in the behavior of some mesoscopic devices like double layer quantum Hall systems [10], where the statistical mechanics of the so called merons analogous to that of the vortices.

In the KTB type transition the bounded dislocation pairs unbind (free dislocations appear in thermal equilibrium) at a certain temperature where an universal jump in shear modulus takes place. As an extension of the KTB theory in the KPV model the effect of applied stress is included additionally through a mean-field type calculation. In the model one of the main results is the recursion equations for the coupling constant and the fugacity which relate to the strength of interaction between dislocations and the average number of dislocations in the system, respectively. Due to the applied external stress the change in fugacity was taken into account in the derivation of the recursion relations and it results in a modified recursion equation for the fugacity in comparison with that of the KTB theory.

However, the stress not only increases the fugacity (and consequently the density of dislocation pairs) but indirectly affects the coupling constant which can be understood as follows. The number of dislocation pairs increases with increasing stress. Larger number of dislocation pairs makes more effective the screening of the interaction between dislocations resulting in a decrease in the coupling constant. It is clear that in a consistent treatment of the effect of the stress one needs to take into account this indirect effect of the stress which was omitted in the KPV model.

The vortex gas in the layered superconductors shows many common aspects with the above discussed dislocation systems in the sense that the character of the interaction between vortices and dislocations can be identical in some cases. The Hamiltonian used in the KPV model is the same as that in the study of the high temperature layered superconductors by taking the 2D limit of the work of [11] for the case of a vortex gas with a current applied uniformly through all layers. This current can be associated with the applied stress in the dislocation systems. Comparing the Hamiltonian of the two models one can identify the corresponding parameters between them. This identification makes possible to obtain the recursion relations for dislocation systems by using the recursion relations found in the case of layered superconductors in the 2D limit (see Pierson’s paper in Ref. [12]). Pierson in his work performed a mathematically rigorous, real-space renormalization group (RG) analysis following the original approach used first by Kosterlitz [13].

Of course, one can derive the recursion equations independently of using the above analogy. Since in Pierson’s work the derivation of the recursion relations are not presented (only the results) we performed the RG analysis with our dislocation systems for clarity. We followed the procedure used in Ref. [12] (the details to be published somewhere else).

In this letter we present a consistent treatment of the dislocation systems in the presence of applied stress. We use the same model as in Ref. [2] (Eq. (1) therein) and give the new recursion relations which includes the effect of the applied external stress both in the fugacity (as in
the KPV model) and in the coupling constant. In our calculations the stress is taken in lowest nonvanishing order both in the equation of the fugacity and the coupling constant. From this study it turns out that the equation for the fugacity remains unchanged (same as the second equation of (4) in Ref. [3]), while in the equation for the coupling constant an additional term proportional to the square of the stress appears. Therefore, our calculations reveal that the indirect effect of the stress modifies only the recursion relation for the coupling constant. However, this latter change has several consequences which will be discussed below.

In the KPV model the stress dependence of the transition temperature is given by a nonlinear implicit equation derived from the stability analysis of the recursion equations (see Eq. (6) in Ref. [3]). Using our new recursion relations a different nonlinear equation is found for the stress dependence of the transition temperature. The above mentioned indirect effect of the stress can be associated precisely. Then, for different materials, we compare the results obtained from the KPV model with that found by using our recursion relations. Qualitative explanations are given for the deviations of the transition temperature from the KPV model. Finally, we summarize the necessary steps for improving the model in order to treat dislocation systems more realistically.

A consistent treatment of the applied stress and the role of the indirect effect of the stress in the dislocation systems are our main subject in this paper. Our results obtained from the extension of the KPV model are a new contribution in this field.

In the frame work of the continuum elasticity theory [7] using the same interaction energy between dislocations as in the KPV model (Eq. (A1) in Ref. [3]) the Hamiltonian of the system $H$ containing $N$ number of dislocations may be expressed as

$$H = -\beta H = 2\pi K_0 \sum_{i<j} p_i p_j G(r_{ij}) + E_0 \sum_i p_i W(r_i) + \ln y_0 \sum_i p_i^2,$$  \hspace{1cm} (1)

where $\beta = 1/k_B T$ and $r_{ij} = r_i - r_j$ is the distance between the $i$th and $j$th dislocation. The summation over pairs $<i,j>$ in the Hamiltonian assumes $i \neq j$ and counts each pair just once. The charge $p_i = +1$ if the Burgers vector at site $i$ is directed to the positive x-axis and equals to $-1$ if it is pointed to the negative x-axis. The charges satisfy the neutrality condition $\sum_i p_i = 0$.

The interactions between dislocations is given by the first term in (1) where

$$G(r) = \ln \left( |r|/a_0 \right)$$  \hspace{1cm} (2)

and $a_0$ is the cut-off radius. The coupling constant in (1)

$$K_0 = \frac{\beta J}{2\pi}$$

and $J = \frac{\mu_0 B_0}{\mu_0 + B_0} \frac{b_0^2}{\pi}$, where $\mu_0$ and $B_0$ are the shear and bulk moduli in the absence of dislocations and $b_0$ is the magnitude of the Burgers vector.

The second term in the Hamiltonian is a sum of the interactions between dislocations and the applied external stress that can be derived from the Peach-Koehler formula [4, 5]. This interaction may be written in such a form that is equivalent to the interaction energy $p_i E r_i$ between the ‘charge’ $p_i$ and the homogeneous external ‘electric field’ $E = \sigma \beta b_0 \hat{x}$, where $\hat{x}$ is the unit vector pointed to the positive x-axis. Then $E_0$ in the Hamiltonian is related to the applied external stress by

$$E_0 = a_0 |E| = \sigma \beta b_0 a_0$$  \hspace{1cm} (3)

and the interaction potential $W$ is given by

$$W(r_i) = \frac{1}{a_0} r_i \hat{x} - \frac{1}{2}.$$  \hspace{1cm} (4)

Note that a constant $-1/2$ has been added to $W$ to be consistent with the definition of the core energy $E_c$ of the dislocation (which must be one half the energy of a dislocation pair at smallest separation and oriented along the direction of the external field $E$).

Finally, in the last term of the Hamiltonian, the fugacity $y_0$ is related to the core energy by

$$\ln y_0 = -\beta E_c + E_0/2,$$  \hspace{1cm} (5)

where the second term is due to the shift of the potential $W$.

It is easy to show that our Hamiltonian is equivalent to that of the KPV model and in this form one can also recognize the resemblance to the Coulomb gas model with applied external electric field. Furthermore, it is clear that the Hamiltonian (1) is similar to that of the model of the layered superconductors if we omit the terms containing $\lambda$ which relates to the interlayer coupling (see Eq. (1) – (3) in Ref. [4]). Below we make a precise correspondence between them.

First, as an extension of the KPV model we derive the recursion equations including the effect of the stress both in the equation of the fugacity and the coupling constant.

A possible starting point for such a calculation is the partition function. Following the procedure used in Ref. [11] one can derive the recursion relations (the details to be published somewhere else).

However, using the above discussed analogy between our dislocation systems and the layered superconductors we may obtain our recursion relations by simple identifying the parameters in the two models via the two Hamiltonians. We found the following correspondences between the two models (the parameters in Ref. [3] are on the left hand side, while our parameters are on the right hand side)

$$\tau \to \alpha, \quad \epsilon \to \lambda, \quad \beta p^2 \to 2\pi K,$$

$$x \to \frac{2}{\pi K} - 1, \quad y \to 2\pi y, \quad J\beta \tau p_i \to E p_i,$$  \hspace{1cm} (6)

(7)
where $J$ does not contain the absorbed factor of $\sqrt{\beta \tau}$ as in Ref. [3] after Eq. (7). Note that $p_{\text{cut}}^2 = 1$ in our case.

Using the above identifications and the recursion relations given in Ref. [3] and omitting the $\lambda$ terms we find for the coupling constant $K$, the fugacity $y$ and $E$

$$
\frac{dK^{-1}}{dl} = 4\pi^2 y^2 \left( 1 + \frac{E^2}{4} \right), \quad (8)
$$

$$
\frac{dy}{dl} = (2 - \pi K + \frac{E}{2}) y, \quad (9)
$$

$$
\frac{dE}{dl} = E. \quad (10)
$$

Eqs. (8)–(10) are our final coupled differential equations with the initial conditions $K(l = 0) = K_0$, $E(l = 0) = E_0$ and $y(l = 0) = \exp(-\beta E_c + E_0/2)$.

The indirect effect of the stress in the coupling constant is reflected by the second term in (8). Omitting the $E^2/4$ term in Eq. (5) we recover the same recursion equations as in the KPV model. The equation for the fugacity given in (3) is the same as in the KPV model. Therefore, the inclusion of the indirect effect of the stress changes only the renormalization of the coupling constant $K$. It is also clear that this indirect effect in $K$ appears in second order in $\sigma$ since $E \sim \sigma$.

At fixed stress the flows obtained from our recursion relations show that below at certain temperature $T_c$ the fugacity $y \to \infty$ and for $T > T_c$ $y \to 0$. The fugacity $y$ is related to the mean density of the unbound dislocation pairs in the system. Increasing the applied stress (note that $E_0 \sim \sigma$) $T_c$ decreases. According to our recursion relations the reason is threefold: (i) the stress increases the fugacity $y_0$, (ii) the last term in Eq. (10) has positive feedback for $y$, (iii) in Eq. (3) the coupling constant $K$ lowers, i.e., the dislocation pairs are more weakly bounded. This latter effect, which is our central issue in this letter, is related to the above mentioned indirect effect of the applied stress.

In the KPV model a nonlinear equation was derived for the stress dependence of the transition temperature by linearizing the recursion equations around the fixed point. Similar way, using Eqs. (3)–(10) we have found that the dimensionless transition temperature $t_c = k_B T_c / J$ is a solution of the following nonlinear equation

$$
t_c = \frac{1 - 2\pi C(E_0) \exp(-\beta E_c + E_0/2)}{4 + E_0}, \quad (11)
$$

where $C(E_0) = \sqrt{1 + \frac{E_0^2}{4}}$, $E_0 = \frac{\sigma b'}{t_c}$

and $\sigma' = \sigma b^2$ is the dimensionless stress while $b'$ is the magnitude of the Burgers vector in units of $a_0$. In the KPV model $C(E_0) = 1$. The indirect effect of the applied stress in Eq. (11) appears via the $E_0^2$ term in $C(E_0)$. The expressions for $t_c$ obtained from the two models differ only by the parameter $C(E_0)$.

To study the role of the indirect effect of the stress as an extension of the KPV model, we solved numerically Eq. (11) for the transition temperature $t_c$ at different values of $\sigma$. We have chosen three particular materials, namely, TiAl, Si and NiAl with the same material parameters as in [3]. According to these parameters the core energies $E_c = 0.25J$ for TiAl, $E_c = 0.78J$ for Si and $E_c = 0.27J$ for NiAl were used. Fig. 1 shows the variation of $t_c$ with the applied stress, $\sigma$ obtained from our calculations and from the KPV model for TiAl and Si. For comparison, the transition temperature is plotted in unit of $J/k_B$, while we used the same stress range for both materials.

![FIG. 1. The transition temperature, $t_c$ as a function of the applied stress, $\sigma$ for TiAl and Si. For parameters see the text. $t_c$ and the stress are units of $J/k_B$ and GPa, respectively. In case of TiAl the solid line and the line with circles correspond to the KPV and our model, respectively. In case of Si the dashed line and the line with squares are the results from the KPV and our model, respectively.](image)

The result from the KPV model can be calculated by simply taking $C(E_0) = 1$ in Eq. (11). It is important to mention that in both the KPV and our model it is assumed that the fugacity, $y_0^2$ $\ll$ 1, i.e., the average density of dislocations is small enough. From our calculation it turns out that for $\sigma < 3.5$ GPa $y_0^2 < 1$. For all the three materials the fugacity was always lower in our model comparing with the KPV model.

From Fig. 1 one can see that the indirect effect of the stress results in a small deviation from the original KPV model for Si, especially for small values of stress. Increasing the stress the differences become larger but it is still about 7% at $\sigma = 3$ GPa. However, the situation for TiAl is changed substantially. Qualitatively, two changes can be seen from the figure. First, the transition temperature is smaller for TiAl than for Si for all values of stress (it is approximately 0.1 smaller at zero stress). Second, the transition temperature calculated from our
model departs from the prediction of the KPV model at lower values of $\sigma$ for TiAl comparing with those for Si. The differences in $t_c$ between our and the KPV model are substantially larger for TiAl than in the case of Si (the difference is about 25 \% at $\sigma = 3$ GPa for TiAl, while only 7\% for Si). We have also calculated the stress dependence of $t_c$ for NiAl. We found that the qualitative feature remains the same as for TiAl and only a slight change can be seen in the values of $t_c$ vs. $\sigma$ (for zero stress $t_c = 0.112$ for NiAl).

The first observation can be understood from the core energy dependence of $t_c$ at zero stress, using Eq. (11). With increasing $E_c$ the transition temperature decreases due to the exponential term in Eq. (11). The physical explanation of this behavior is as follows. For large $E_c$ the number of thermally activated dislocations is relatively small. This implies that the screening of the dislocation pairs by other dislocations is weaker. The coupling strength (normalized by $J$) between pairs remains strong. Hence, the unbounding of the pairs, which is related to the phase transition, takes place at higher temperature. The core energies for TiAl and NiAl are approximately the same, while for Si it is much larger. Thus, $t_c$ will be higher for Si than TiAl and for NiAl it is nearly the same as that for TiAl.

The second observation is less obvious. Again, the analysis of the core energy dependence of $t_c$ shows that at lower $E_c$ the indirect effect of the stress becomes more prominent. The parameter $C(E_0)$ in Eq. (11) can be dominant besides the suppression of the exponential term. On the other hand, with increasing stress, $t_c$ obtained from our model is always lower than that predicted from the KPV model independently from the value of $E_c$. The physical reason is that at higher $\sigma$ the so-called ‘electric field’ makes weaker the bounds between the dislocation pairs. In Eq. (11) it is reflected by the second term. This term is entirely the consequence of the indirect effect of the stress.

In the KPV model the Burgers vector has only two possible orientations correspondingly +1 and −1 charges. However, in a solid there can be more orientations of the Burgers vector depending on the crystal structure. It is desirable to extend the model in order to take into account the possible Burgers vector systems in the crystal. In the present study (and also in the KPV model) the role of the angular dependent force between dislocations has not been considered. The quantitative behavior of the stress dependence of the transition temperature is likely to influence by this force. Some preliminary work on these directions have already been made.

The KPV model has been applied to the brittle-to-ductile transition and the deformation of whiskers in Ref. [8]. We believe that our model contributes to a better understanding of these two phenomena.

In conclusion, we present an extension of the KPV model by taking into account the indirect effect of the applied external stress on the solid. Realizing the analogy between our dislocation systems and the layered superconductors we derive the correspondig recursion equations. From these equations we obtain a nonlinear equations for the transition temperature. The implication of our model is discussed in the case of three particular materials. In general, we find that the indirect effect of the stress in $T_c$ plays crucial role in some materials depending on their core energies.

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