FIRST ORDER IN 2D DISCLINATION MELTING

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We present a Monte Carlo study of a 2D gas of crystal disclinations and find a first-order melting transition.

In recent years there has been considerable progress in understanding the phase transitions of crystal melting via the statistical mechanics of crystalline defects [‡1]. At sufficiently high temperatures these can proliferate, thereby destroying the translational and rotational order. In three dimensions, it was found that the first order of the melting transition is caused by an interplay of dislocations and disclinations [2]. In a crystal, disclinations are bound permanently in pairs by a linear potential, and such pairs can be observed as dislocations. Above a certain temperature, these bound pairs proliferate. The proliferation causes a screening of the elastic forces (a crystalline version of the Meissner effect [3]) which weakens the attraction between the constituent disclinations from R to $1/R$ and allows them to unbind. The joint process, proliferation of pairs plus unbinding, is what makes the transition first order [2]. The theoretical analysis was confirmed by a Monte Carlo study of a three-dimensional model on a simple cubic lattice (with spacing a)

$$Z = \int_{-\pi}^{\pi} \prod_{x,i} \frac{\mathrm{d}A_i}{2\pi} \exp\left[\beta\left(\sum_{x,i<j} \cos(\nabla_i A_j + \nabla_j A_i) + 2\xi \sum_{x,i} \cos(\nabla_i A_i)\right)\right], \tag{1}$$

where $\beta = \mu a^3/(2\pi)^2 T$ with μ = shear module. We neglect the Lamé constant λ for simplicity and allow for a non-isotropic crystal via the elastic constant ξ. At $\beta_{\mathrm{melt}} = 0.76$ there is a first-order transition with a transition entropy $\Delta s = 1.4$/site. This β_{melt} corresponds to a Lindemann parameter $L \approx 143\sqrt{\beta_{\mathrm{melt}}} \approx 125$ in good agreement with experimental values.

That this model describes an ensemble of crystal defects had been shown previously by duality transformations [5,6].

In two dimensions, a similar study is still missing. According to Halperin and Nelson [7], defect melting should be a sequence of two continuous Berezinskii–Kosterlitz–Thouless [8] transitions. The crystalline phase contains bound pairs of dislocations. At a certain critical temperature, these become separated and the crystal enters into a mesophase with no translational but orientational order ("hexatic phase"). If heated further, there is another transition in which dislocations split up into disclinations.

Unfortunately, these conclusions were found to contradict Monte Carlo simulations of two-dimensional atomistic models which always display a first-order transition [9]. This stimulated a direct Monte Carlo study of a gas of dislocation vectors, by Saito, with the partition function [10]

$$Z = \sum_{\{b_i(x)\}} \exp\left(-(2\pi)^2\beta \sum_{x,x'} b_i(x) V_{ij}(x-x') b_j(x') - e_c \sum_x b_i(x)^2\right), \tag{2}$$

[‡1] This view dates back to Shockley [1].

where $V_{ij}(x-x')$ is the lattice version of the transverse Coulomb potential

$$(\delta_{ij}\nabla\bar{\nabla}-\nabla_i\bar{\nabla}_i)/(\nabla\bar{\nabla})^2 \approx -(4\pi)^{-1}(\delta_{ij}\log r - x_i x_j/r^2)+\dots . \tag{3}$$

Saito found that for a slightly negative core energy e_c, the transition was definitely first order.

At this point it was recognized [11] that there was something unphysical about the core energy $E_c = e_c \Sigma b_i(x)^2$. It had been introduced into the model by Halperin and Nelson in order to use the fugacity expansion as in Kosterlitz and Thouless' work. In a real crystal, however, all defects may be viewed as superpositions of dislocations alone. In this case, such a simple core energy cannot by present: In order to see this we observe that the gauge field of stress couples only to the transverse projection of b_i ($b_i^{\mathrm{T}} = (\delta_{ij}-\nabla_i\bar{\nabla}_j/\nabla\bar{\nabla})b_j$). This is why linear elasticity can give only an energy associated with this projection of b_i. Moreover, neither non-linear elastic energies which go with higher powers in the stress tensor nor higher derivative energies can produce the above form of E_c. Whatever the short distance forces, they have to respect an elementary property of crystalline defects: When stacking up a string of dislocations along the positive x_1 or x_2 axis,

$$b_1 = 0, \quad b_2 = \epsilon\theta(x_1)\delta(x_2), \tag{4}$$

or

$$b_1 = -\epsilon\theta(x_2)\delta(x_1), \quad b_2 = 0, \tag{5}$$

the two configurations are physically indistinguishable. They correspond to a single disclination sitting at the origin, once created by a Volterra cut along the x_1 and once along the x_2 axis. Both cuts yield the *same* disclination. This is analogous to the physical irrelevance of the Dirac string emerging from a magnetic monopole which can be chosen to lie anywhere in space [12]. A simple core energy Σb_i^2 would give an infinite energy to either string and thus prevent the pileup of dislocations to disclinations which is essential to the melting process [11]. Saito's choice of a very small negative core energy removed this unphysical feature of Halperin and Nelson's ansatz for E_c and this explains why he was able to observe a proper first-order melting transition into an isotropic liquid.

In the new model of melting, eq. (1), the interrelation between dislocations and disclinations is automatically incorporated. In order to see this, let us perform a Villain approximation

$$Z = \left(\frac{I_0(\beta)}{\sqrt{2\pi\beta_v}}\right)^N \left(\frac{I_0(2\xi\beta)}{\sqrt{4\pi\xi_v\beta_v}}\right)^{2N}$$

$$\times \sum_{\{n_{11},n_{12},n_{22}\}} \int_{-\pi}^{\pi} \prod_{x,i} \frac{\mathrm{d}A_i}{2\pi} \exp\left[-\tfrac{1}{2}\beta_v \sum_x \left((\nabla_1 A_2 + \nabla_2 A_1 - 2\pi n_{12})^2 + 2\xi_v \sum_i (\nabla_i A_i - 2\pi n_{ii})^2\right)\right], \tag{6}$$

where $\beta_v = -\{2\log[I_1(\beta)/I_0(\beta)]\}^{-1}$ and $2\xi_v\beta_v = -\{2\log[I_1(2\xi\beta)/I_0(2\xi\beta)]\}^{-1}$ and n_{ij} are integer numbers.

A quadratic completion gives then the integrand

$$\int \frac{\mathrm{d}\sigma_{12}}{\sqrt{2\pi\beta_v}} \frac{\mathrm{d}\sigma_{11}\mathrm{d}\sigma_{22}}{4\pi\xi_v\beta_v} \exp\left(-\frac{\sigma_{12}^2}{2\beta_v} - \frac{\sigma_{11}^2+\sigma_{22}^2}{4\beta_v\xi_v} + \mathrm{i}\sigma_{12}(\nabla_1 A_2 + \nabla_2 A_1 - 2\pi n_{12}) + \mathrm{i}\sum_i \sigma_{ii}(\nabla_i A_i - 2\pi n_{ii})\right), \tag{7}$$

which after a sum over n_{ij} and an integral over A_1, A_2 becomes a sum over integer valued stress field $\bar{\sigma}_{ij}$

$$(\sqrt{2\pi\beta_v}4\pi\xi_v\beta_v)^{-1} \sum_{\{\bar{\sigma}\}} \delta_{\bar{\nabla}_j\bar{\sigma}_{ji},0} \exp\left[-\frac{\bar{\sigma}_{12}^2}{2\beta_v} - \frac{\bar{\sigma}_{11}^2+\bar{\sigma}_{22}^2}{4\beta_v\xi_v}\right]. \tag{8}$$

The conservation law $\bar{\nabla}_j\bar{\sigma}_{ji} = 0$ is enforced by introducing a stress gauge field χ [‡2] with $\bar{\sigma}_{ij} = \epsilon_{ik}\epsilon_{jl}\bar{\nabla}_k\bar{\nabla}_l\chi$ which is

[‡2] Actually, the case of $D = 2$ dimensions is degenerate in that χ is not really a gauge field. Only in higher dimensions it is. For example, if $D = 3$, $\bar{\sigma}_{ij} = \epsilon_{ikl}\epsilon_{jmn}\bar{\nabla}_k\bar{\nabla}_m\chi_{ln}$ and χ_{ln} is a proper gauge field with $\bar{\sigma}_{ij}$ being gauge invariant under $\chi_{ln} \to \chi_{ln} + \nabla_l\varphi_n + \nabla_n\varphi_l$.

made integer by a sum over integer numbers m. This gives

$$\int_{-\infty}^{\infty} \prod_x \mathrm{d}\chi \exp\left(-(2\beta_v)^{-1} \sum_x (\nabla_1 \nabla_2 \chi)^2 - (4\beta_v \xi_v)^{-1} \sum_x [(\nabla_1^2 \chi)^2 + (\nabla_2^2 \chi)^2]\right) \sum_{\{m(x)\}} \exp\left(\mathrm{i} \sum_x 2\pi m \chi\right). \quad (9)$$

Integrating out the gauge fields shows that $m(x)$ interact via a Boltzmann factor

$$\exp\left(-(4\pi)^2 \beta_v \xi_v \sum_{x,x'} m(x) v(x-x') m(x')\right), \quad (10)$$

with

$$v(x-x') = [(\nabla\bar{\nabla})^2 + 2(\xi_v - 1)\nabla_1 \bar{\nabla}_1 \nabla_2 \bar{\nabla}_2]^{-1}(x, x').$$

Hence the ensemble of integer charges $m(x)$ behaves like a gas of disclinations in an anisotropic crystal.

Some qualitative features of such a gas were discussed recently by Nelson [14]. For low temperatures, the disclinations are bound together in quartets which can be interpreted as pairs of dislocations. If quartets split into doublets, each doublet looks like a single dislocation. These dislocations can split further into individual disclinations. Guided by the analysis of Nelson and Halperin, Nelson concluded that these processes should take place in a sequence of two continuous phase transitions. This would contradict our qualitative analysis [12].

In order to find out what really happens, we have investigated the gas of defects via Monte Carlo techniques using directly our model eq. (1), with lattices varying in size from 30 X 30 to 60 X 60 sites with periodic boundary conditions. The continuous variables $A_1, A_2 \in (-\pi, \pi)$ were approximated by 16 equidistant points. The thermodynamic behavior was studied in the same way as in the three-dimensional model [4]. We started out from a small value of β in the crystalline phase and established equilibrium by going through a few iterations. Then we decreased

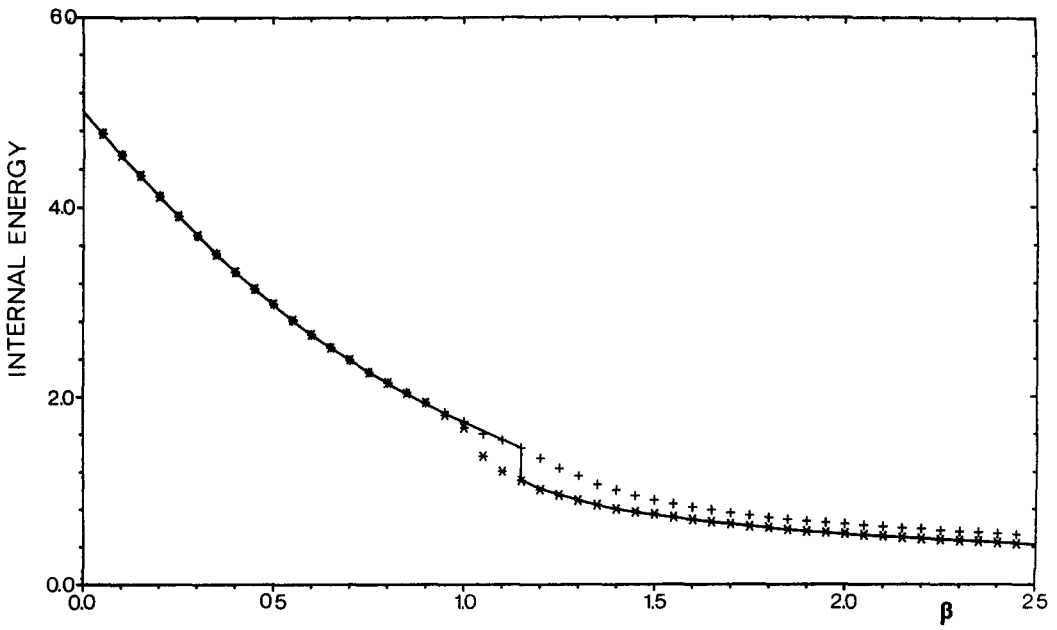

Fig. 1. The internal energy of the model (1) on a 60 X 60 square lattice, $u = -N^{-1}\,(\partial/\partial\beta) \log Z$, as a function of β as obtained in a thermal cycle and after long equilibration runs close to β_{melt}. For the equilibration procedure see the text. We see that $\Delta u \approx 0.26 \pm 0.05$ and $\Delta s = \beta_{\mathrm{melt}} \Delta u = 0.3 \pm 0.05$.

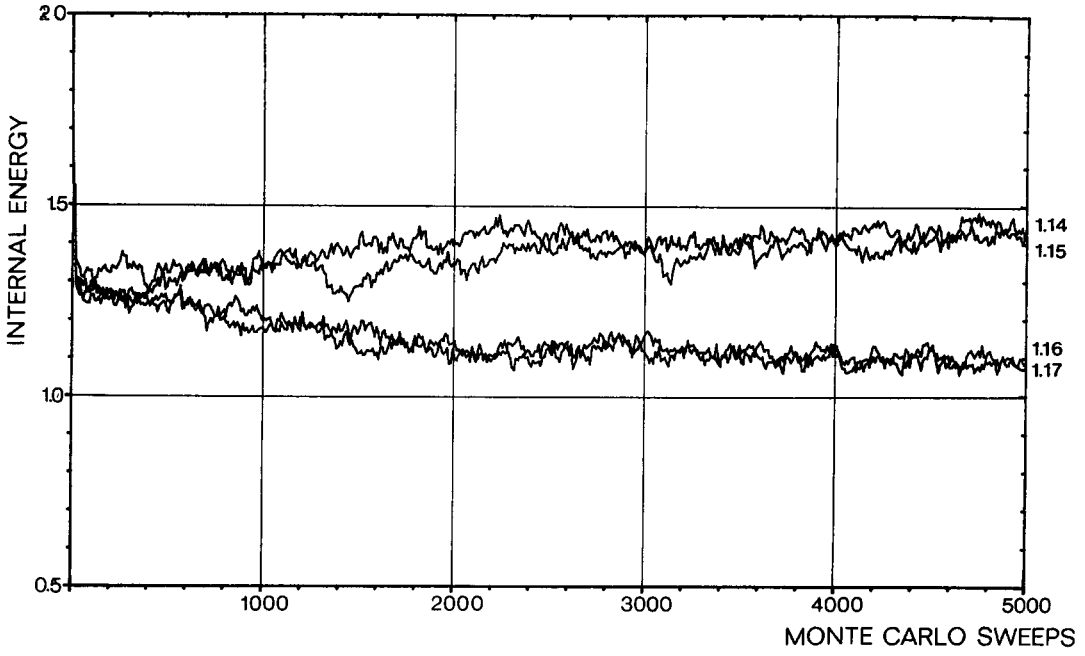

Fig. 2. The behavior of the internal energy on a 60 X 60 square lattice in the immediate neighborhood of $\beta_{melt} \approx 1.15$ for many iterations starting with a mixed state.

successively the inverse temperature by steps $\Delta\beta = 0.05$ and repeated at each step the equilibriation process 20 times after which we measured the internal energy averaging over 40 further iterations. After reaching the disordered state at very high temperature, we run backwards to low temperatures. The energy curve obtained in this way shows a pronounced hysteresis with considerable undercooling suggesting a first-order transition (see fig. 1) [‡3].

The precise behavior in the neighborhood of the transition was studied via the development of a mixed state over many iterations (5000), as shown in fig. 2 for the special case $\xi = 1$. This led to the internal energy plotted as

[‡3] This result is in agreement with a first independent exploratory Monte Carlo run by H. Bohr who also found a hysteresis.

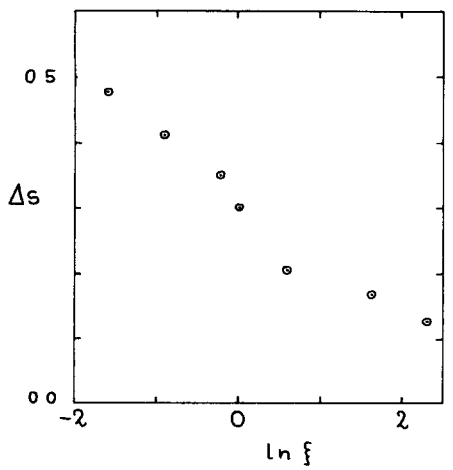

Fig. 3. The entropy jump $\Delta s = \beta_{melt}\Delta u$ as a function of the anisotropy parameter ξ.

the continuous line in fig. 1 and permitted a precise localization of the transition temperature. On the 60×60 lattice, we find $\beta_{melt} \approx 1.15$ with a jump in the internal energy $\Delta u \approx 0.26 \pm 0.05$. The corresponding transition entropy $\Delta s = \beta_{melt} \Delta u \approx 0.3 \pm 0.05$ per atom (in units of k_B) is of the same size as in atomistic simulations [9]. For $\xi \neq 1$ the curves are quite similar. The entropy jump depends on ξ as shown in fig. 3.

It is interesting to point out that, at the mean field level, the point $\xi = 1$ is tricritical [15], with the transition being first order for $\xi < 1$ and second order for $\xi > 1$. This is due to the quartic term in the field theory changing sign at that point. The fluctuation corrections, however, generate (from the higher powers in the field) a negative quartic potential for all physically acceptable ξ values, such that the transition does remain first order, just as anticipated by the general analysis in ref. [11].

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