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Dislocations in the ground state of the solid-on-solid model on a disordered substrate

Frank O Pfeiffer† and Heiko Rieger†‡

† Institut für Theoretische Physik, Universität zu Köln, 50937 Köln, Germany
‡ Institut für Theoretische Physik, Universität des Saarlandes, 66041 Saarbrücken, Germany

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Abstract. We investigate the effects of topological defects (dislocations) to the ground state of the solid-on-solid (SOS) model on a simple cubic disordered substrate utilizing the min-cost-flow algorithm from combinatorial optimization. The dislocations are found to destabilize and destroy the elastic phase, particularly when the defects are placed only in partially optimized positions. For multi-defect pairs their density decreases exponentially with the vortex core energy. Their mean distance has a maximum depending on the vortex core energy and system size, which gives a fractal dimension of 1.27 ± 0.02. The maximal mean distances correspond to special vortex core energies for which the scaling behaviour of the density of dislocations change from a pure exponential decay to a stretched one. Furthermore, an extra introduced vortex pair is screened due to the disorder-induced defects and its energy is linear in the vortex core energy.

1. Introduction

At low temperatures the physics of crystal surfaces on disordered substrates is dominated by the randomness rather than thermal fluctuations. In (2 + 1)-dimensions this elastic surface is expected to have a roughening phase transition at a critical temperature T_c from a thermally *rough* phase for $T > T_c$ to a *super-rough* phase for $T < T_c$ [1–3], corresponding to a height–height correlation function $\log(r)$ and $\log^2(r)$ respectively. The $\log^2(r)$-super-rough behaviour was numerically confirmed at finite temperature via Monte Carlo simulations [4] as well as in the limit of a vanishing temperature via exact ground state calculation using combinatorial optimization methods [5–7].

In this paper, we study the stability of the low-temperature (glassy) phase of the solid-on-solid model (SOS) on a disordered substrate [7–9] with respect to the formation of topological point-like defects. We also consider the density of defects and the screening effect of pre-existing pairs to an introduced extra pair and allow for a vortex core energy.

The SOS model on a disordered substrate is given by the uniformly distributed *substrate* height $d_i \in [0, 1]$ and the integer *crystal* height n_i on a simple cubic $L \times L$ ¤¤lattice G with periodic BC and lattice site i as schematically shown in figure 1. The $h_i = n_i + d_i$ denotes the *total surface* height at site i and the SOS model Hamiltonian is defined by

$$H = \sum_{\langle ij \rangle} (h_i - h_j)^2 \tag{1}$$

where the sum runs over all nearest-neighbour pairs $\langle ij \rangle$. To calculate the ground state of the SOS Hamiltonian (1) we introduce the *crystal* height-differences $n^*_{ij} = n_i - n_j$ (integer) and

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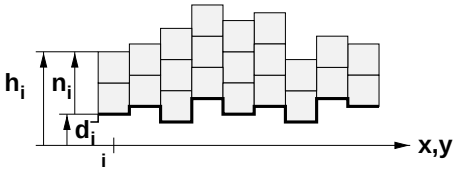

Figure 1. Height profile $h_i = n_i + d_i$ in the (2 + 1) SOS model, where $d_i \in [0, 1]$ are the random offsets of the disordered substrate and n_i the crystal heights (arbitrary integers) on the lattice site i.

substrate height-differences $\boldsymbol{d}^*_{ij} = d_j - d_i$ ($\in [-1, +1]$) along the links $k = (i, j)$ on the dual lattice G^*. Thus we get the following SOS Hamiltonian for the dual space:

$$H(\{\boldsymbol{n}^*_k\}) = \sum_k (\boldsymbol{n}^*_k - \boldsymbol{d}^*_k)^2. \tag{2}$$

The minimal (optimal) energy configuration $\{\boldsymbol{n}^*_k\}_{\min}$ will just be the closest integer $\boldsymbol{n}^*_k$ to $\boldsymbol{d}^*_k$ for all links $k = (i, j)$. On the other hand, since the $\boldsymbol{n}^*_k$ describe height-differences in the scalar field given by the n_i their sum along any oriented cycle on the surface around site i has to be zero, i.e. the lattice divergence of $\boldsymbol{n}^*$ has to vanish for each site i:

$$(\nabla \cdot \boldsymbol{n}^*)_i = 0. \tag{3}$$

Note that n_i can be considered to be a potential and $\boldsymbol{n}^*_{ij}$ as its force field. Obviously, for a typical disordered substrate the minimal configuration $\{\boldsymbol{n}^*_k\}_{\min}$ violates the mass balance constraint (3). Figure 2 shows an example of a disordered substrate with substrate height $d_i = 0.0, 0.2, 0.4$ and 0.6. Consider the differences $\boldsymbol{d}^*_k$: across the dashed line we have $\boldsymbol{d}^*_k = 0.6$ and $|\boldsymbol{d}^*_k| < 0.5$ elsewhere. Consequently, the absolute minimum-energy configuration without any balance constraint is given by $\boldsymbol{n}^*_k = 1$ and $\boldsymbol{n}^*_k = 0$ respectively. With respect to the balance constraint (3) the only feasible optimal solution (ground state) is a flat surface, i.e. $\boldsymbol{n}^*_k = 0$ for all links $k = (i, j)$. On the other hand, dislocations of Burgers charge† b can be introduced if one treats the height field h_i as a multi-valued function which may jump by b along lines that connect two point defects (i.e. a dislocation pair) [10]. Therefore, for the given example (figure 2) it should be clear that the minimal configuration $\{\boldsymbol{n}^*_k\}_{\min}$ (see above) is exactly the optimal (i.e. ground state) configuration with one dislocation pair. One of the two defects has a Burgers charge $b = +1$ and the other one $b = -1$. The pair is connected by a dislocation line (dashed line in figure 2) along which one has $\boldsymbol{n}^*_i = 1$. This already demonstrates that due to the disorder the presence of dislocations decreases the ground state energy and a proliferation of defects appears. Alternatively, in [7] a dislocation pair (excited step) was introduced by fixing the boundary to zero and one.

2. Defect pairs in the SOS model

The defect pairs in the disordered SOS model are source and sink nodes of strength $+b$ and $-b$, respectively, for the network flow field n_i [8,9], which otherwise fulfils $(\nabla \cdot \boldsymbol{n}^*)_i = 0$, i.e. we have to modify the mass balance constraint (3) as follows:

$$(\boldsymbol{\nabla} \cdot \boldsymbol{n}^*)_i = \begin{cases} 0 & \text{no dislocation at} \quad i \\ \pm b & \text{dislocation at} \quad i. \end{cases} \tag{4}$$

† $b = |\boldsymbol{b}|$, where $\boldsymbol{b}$ is the Burgers vector.

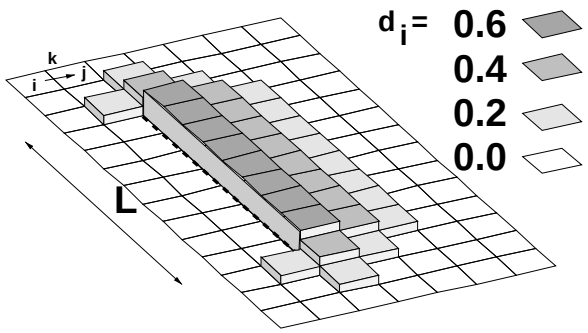

Figure 2. Example of a disordered substrate, heights d_i, in a random-surface model with a single dislocation pair connected along a straight line of size L (dashed line). The optimal surface without dislocations would be flat, i.e. $n_i = 0$ for all sites i; however, allowing dislocations would decrease the ground state energy (see the text).

Thus the ground state problem is to minimize the Hamiltonian (2) subjected to the mass balance constraint (4) which can be solved by the successive-shortest-path algorithm [6, 8, 9]. In the following we concentrate on defect pairs with $b = \pm 1$.

The defect energy ΔE is the difference of the minimal energy configuration *with* and *without* dislocations for each disorder realization, i.e. $\Delta E = E_1 - E_0$. More precisely, for the configuration *with* N defect pairs of Burgers charge $b = \pm 1$ we introduce two extra nodes s and t with $n_s = +N$ and $n_t = -N$ respectively and connect them via external edges or bonds with particular sites of the lattice depending on the degree of optimization: (a) with two sites separated by $L/2$ (figure 3(*a*)), (b) the source node with one site i and the sink node with the sites on a circle of radius $L/2$ around i (figure 3(*b*)) and (c) both nodes with the whole lattice. Case (a) corresponds to a *fixed* defect pair, (b) to a *partially optimized* pair along a circle, both separated by a distance $L/2$, and (c) to a *completely optimized* pair with an arbitrary separation. In all cases the energy costs for flow along these external edges are set to a positive value in order to ensure the algorithm to find the optimal defect pair on the chosen sites. These 'costs' have no contribution to the ground state energy. In the case of *multi-pairs* we always use graph (*c*). Here, the optimal number N of defects in the system is gradually determined starting with one pair ($N = 1$) with a vortex core energy $2E_c$ and checking whether there is an energy gain or not. If yes, add a further pair (with $2E_c$) and repeat the procedure until there is no energy gain from the difference of the ground state energy between two iterations.

3. Single-defect pair ($N = 1$)

We study the defect energy ΔE and its probability distribution $P(\Delta E)$ on a $L \times L$ lattice with $L = 6$, 12, 24, 48, 96 and 192 and 2×10^3–10^5 samples for each size and consider the three cases (a)–(c) (see above). With an increasing degree of optimization a negative defect energy ΔE becomes more probable and its probability distribution $P(\Delta E)$ differs more and more from the Gaussian fit, figure 4. The resulting disorder-averaged defect energy $[\Delta E]_{\rm dis}$ scales as

$$[\Delta E]_{\rm dis} \sim \begin{cases} \ln(L) & \text{fixed defect pair} \\ -0.27(7) \times \ln^{3/2}(L) & \text{partially optimized} \\ -0.73(8) \times \ln^{3/2}(L) & \text{completely optimized} \end{cases} \tag{5}$$

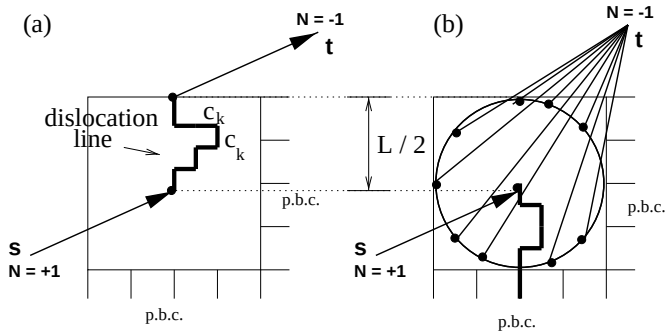

Figure 3. Graph of a $L \times L$ lattice with periodic BC for the implementation (*a*) of one *fixed* defect pair and (*b*) of a *partially optimized* pair. Both are separated by $L/2$. The energetic costs are $c_k(\boldsymbol{n}_k^*) = (\boldsymbol{n}_k^* - \boldsymbol{d}_k^*)^2$ at the dual site $k = (i, j)$. Dislocations are induced by two extra nodes s and t, which are connected with the possible positions of the defects (big dots).

and its related variance σ as

$$\sigma(\Delta E) \sim \begin{cases} \ln(L) & \text{fixed defect pair} \\ \ln^{2/3}(L) & \text{partially optimized} \\ \ln^{1/2}(L) & \text{completely optimized} \end{cases} \tag{6}$$

where the exponents are approximations for the best data collapse. The defect energy indicates that for the optimized cases dislocations can proliferate due to thermal fluctuations and melt the elastic super-rough phase. Furthermore, for a growing degree of optimization the scaling amplitude of $[\Delta E]_{\text{dis}}$ increases.

The mean length (mass) l_{DL} of the line connecting the two defects scales with the system size L according to the fractal dimension

$$d_f = 1.28 \pm 0.02 \tag{7}$$

for the *fixed* and *partially optimized* situation. This value is close to the fractal dimension of an optimal path in a disordered environment [11] $d_f^{\text{opt.path}} = 1.20 \pm 0.02$ in $d = 2$), but still significantly different from it. Although at first sight there might be similarities between this problem and the situation considered here (at least for *fixed* position of the defect pair) there are differences that are significant enough (e.g. the underlying energy costs for the defect situation are not uncorrelated) to put them both in different universality classes.

For the *completely optimized* case figure 5 shows a probability distribution $P(l_{DL})$, which behaves as

$$P_L(l_{DL}) \sim \frac{1}{L} \times p\left(\frac{l_{DL}}{L}\right). \tag{8}$$

4. Multi-defect pairs ($N > 1$)

Next, we study the effect of a uniformly given vortex core energy E_c to the system of *multi-defect pairs* ($N > 1$) as a simplification of the real situation with a distribution of E_c. As shown in figure 6(*a*), the density ρ of defects decays exponentially with an increasing E_c, i.e.

$$\rho(E_c) \sim e^{-(E_c/E_0)^\alpha}. \tag{9}$$

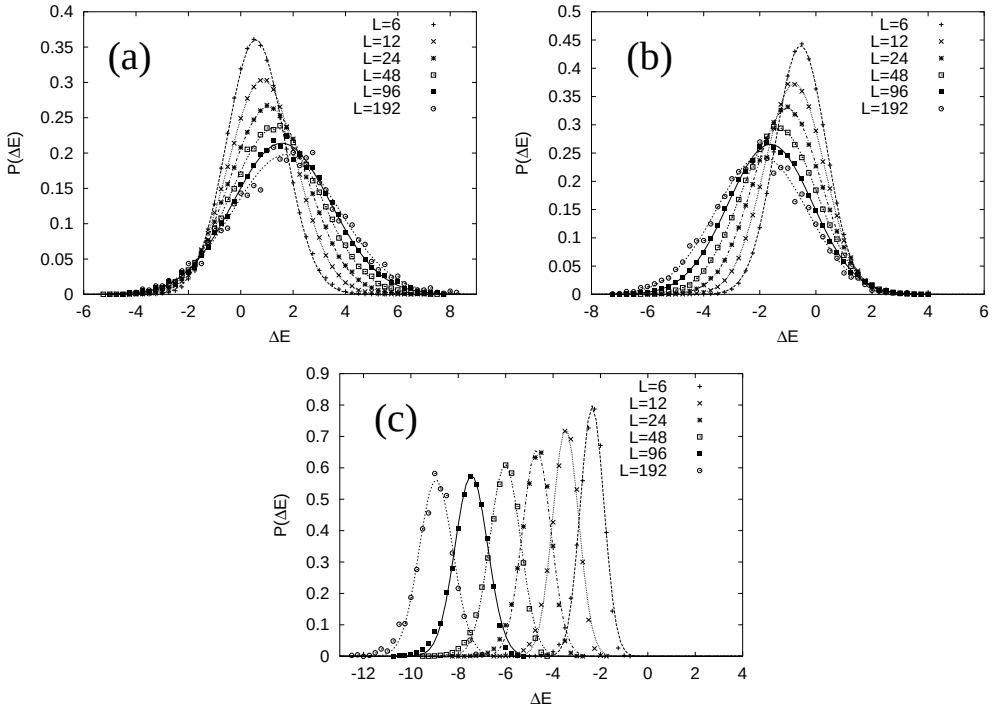

Figure 4. Probability distribution $P(\Delta E)$ of a large-scale topological excitation with a Gaussian fit for different optimizations: (*a*) for a *fixed* defect pair, (*b*) for a *partially optimized* pair and (*c*) for a *completely optimized* pair with different system sizes L.

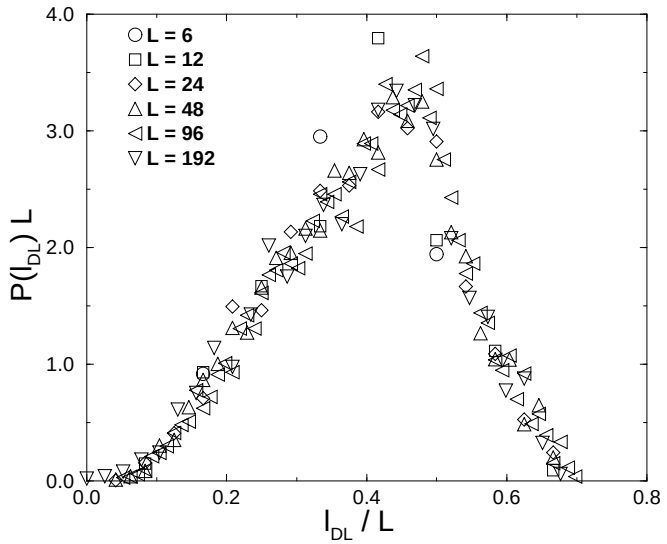

Figure 5. Finite-size-scaling relation of the probability distribution $P(l_{DL})$ of the mean distance l_{DL} between two optimally placed dislocations for system size $L = 6$, 12, 24, 48, 96 and 192. The data collapse for $P_L(l_{DL}) \sim 1/L \times p(l_{DL}/L)$.

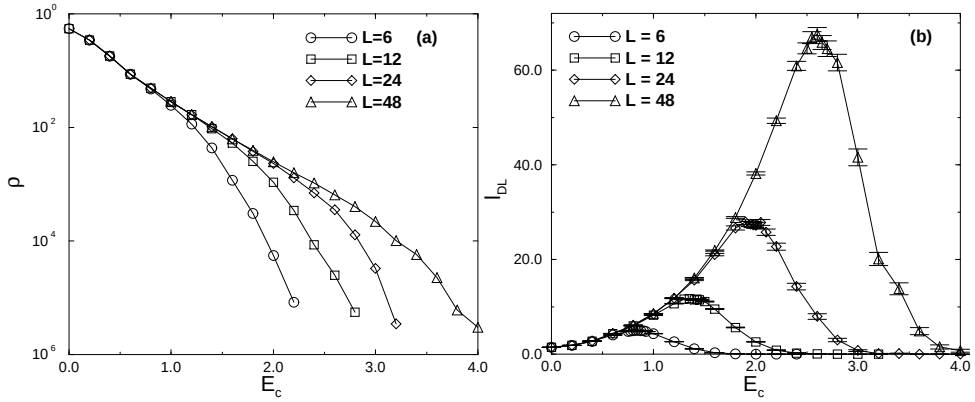

Figure 6. (*a*) Density ρ of defects with respect to the vortex core energy E_c for different system sizes $L = 6$–48 and 10^3 up to 10^4 samples. The log–lin plot indicates an exponential decay of ρ. Simultaneously, (*b*) the mean distance l_{DL} of all dislocation pairs versus the vortex core energy E_c. Comparing (*a*) and (*b*) one sees that the maximal length l_{DL} occurs at the cross-over energy $E_c^{\max}$ (see the text).

For the E_0 and α we can distinguish between two intervals of E_c which refer to a stretched and a pure exponential decay, respectively. In detail we have the following values:

$E_c \in$	E_0	α
$[0, \infty[$	0.6 ± 0.15	0.75 ± 0.2
$[0, E_c^{\max}(L)[$	0.45 ± 0.03	1

The upper limit ${E_c}^{\max}(L)$ corresponds to the maximal mean length l_{DL} for each system size L, cf figures 6(*a*) and (*b*), and scales as

$$ {E_c}^{\max} \approx (\text{const.} + 0.47 \pm 0.02) \times \ln(L))^{3/2}. \tag{10} $$

Moreover, we found the same scaling behaviour for the vanishing defect energy, i.e. $[\Delta E]_{\text{dis}} = 0$:

$$ E_{c0} \approx (\text{const.} + (0.47 \pm 0.01) \times \ln(L))^{3/2}. \tag{11} $$

From the plot of the maximal mean length l_{DL} (figure 6(*b*)) versus the system size L, i.e. $l_{DL}(E_c^{\max}) \sim L^{d_f}$, the fractal dimension d_f is given by

$$ d_f = 1.27 \pm 0.07 \tag{12} $$

which agrees (within error bars) with the value for the single line situation reported in equation (7).

Finally, we focus on the effect of introducing an *extra* fixed defect pair separated by $L/2$ to an already (completely) optimized configuration with a vortex core energy E_c. This extra pair costs

$$ \Delta E_{\text{fix}} = E_1' + 2E_c - E_1 \tag{13} $$

where E_1 denotes the ground state energy for N (pre-existing optimal) pairs and E_1' the energy for $N + 1$ optimally placed pairs, both for the same disorder configuration $\{d_i\}$. As plotted in figure 7, ΔE_{fix} is constant in L, but linear in E_c, i.e.

$$ \Delta E_{\text{fix}}(L) = (0.17 \pm 0.02) + (4.35 \pm 0.02) \times E_c. \tag{14} $$

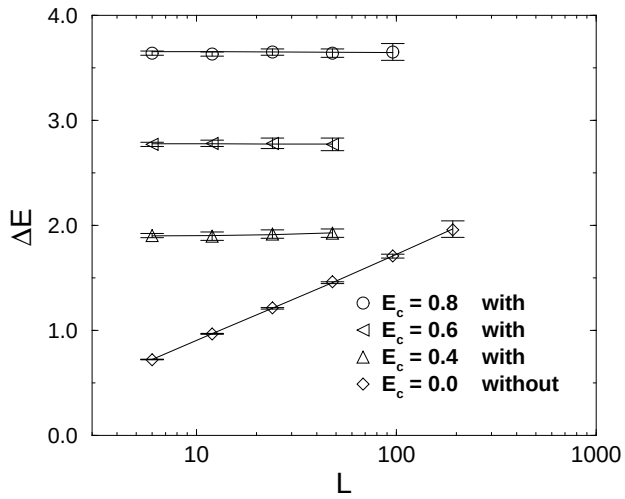

Figure 7. Defect energy ΔE of a single (introduced) defect pair versus the system size L ($L = 6$, 12, 24, 48, 96) in a system *with* and *without* an already optimal number of dislocations for different vortex core energies E_c.

Thus, one obtains a screening effect of the defect–defect interaction due to disorder-induced dislocations. In comparison, figure 7 also shows the case for a single pair ($N = 1$) *without* pre-existing pairs as studied in section 3.

5. Related models

A similar picture of the effect of dislocations to a randomly pinned elastic media at $T = 0$ were found for other discrete models: the *fully-packed loop* (FPL) model [12] and the matching model [14], both on a bipartite hexagonal lattices with a linear energetic cost function and periodic BC

In the case of a single *fixed* defect pair we found the same $\ln(L)$ behaviour of the defect energy as for the excitation step in [7, 12], but got a smaller fractal dimension $d_f = 1.28(2)$ rather than $d_f = 1.35(2)$ [7]. The disorder-induced dislocations turned out to destroy the quasi-long-range order of the elastic phase due to a negative scaling behaviour of defect energy ΔE with respect to L for optimally placed defects, i.e. $\Delta E \sim -\ln^{3/2}(L)$, in good agreement with the results of the FPL model [12]. When taking into account screening and a uniform vortex core energy E_c in addition to the energy balance ΔE, one finds that the energetic costs $\Delta E_{\rm fix}$ of an introduced fixed pair does not depend on the system size L, as shown for the FPL [13] and matching [14] model. In addition, we found for the disordered SOS model a linear dependence of $\Delta E_{\rm fix}$ on the vortex core energy E_c (figure 7). One concludes that this extra pair is screened by the pre-existing defect pairs. For the exponentially decay of density ρ of the dislocation pairs we distinguished between (a) the whole range of the vortex core energy E_c and (b) a range with an upper limit $E_c^{\max}(L)$, for which (latter case) the mean defect length l_{DL} was found to be maximal. Case (a) corresponds to $\alpha = 1$ and $E_0 = 0.45(3)$ and the maximal length l_{DL} related to the cross-over energy $E_C^{\max}(L)$ behaves as $l_{DL} \sim L^{d_f}$ with the fractal dimension $d_f = 1.267(7)$. Both results were also found in [14]. For case (b) we get $\alpha \approx 0.75$ (close to $\frac{2}{3}$) and $E_0 \approx 0.6$ in good agreement with [13].

Finally, we relate the SOS model (1) to the continuum description of a randomly pinned elastic medium on large length scales given by the *sine–Gordon* model Hamiltonian

$$H = \int \mathrm{d}^2 \boldsymbol{r} \left[\frac{K}{2} (\nabla u(\boldsymbol{r}))^2 - w \cos(2\pi (u(\boldsymbol{r}) - d(\boldsymbol{r}))) \right] \tag{15}$$

where K is the elastic constant and $d(\boldsymbol{r})$ a random field out of [0,1]. The first term represents the elastic energy E_{el} and the second one the random pinning energy E_{pin}. The model is known to describe a weakly disturbed vortex lattice in a thin two-dimensional superconducting film introduced by a parallel field [15–17]. Other experimental realizations are charge density waves [18] and Wigner crystallization of electrons [19].

The relation to the SOS model is as follows: in the limit of an infinite coupling strength $w \to \infty$ and $T = 0$ the *sine–Gordon* model maps onto a lattice SOS model equation (1), as the cosine term of equation (15) forces the displacement field $u(\boldsymbol{r})$ to be $u(\boldsymbol{r}) = d(\boldsymbol{r}) + n(\boldsymbol{r})$ [4, 9, 21], where $n(\boldsymbol{r})$ is an integer. One can identify the $u(\boldsymbol{r})$ as the continuous height field $h(\boldsymbol{r})$ of the SOS model.

The results of the analytical study of the *sine–Gordon* model [12, 20, 22] are in good agreement with our results, but only refer to the cases of *fixed* and *completely optimized* pairs. Furthermore, these studies allow another interpretation of the defect energy ΔE and density ρ. From the calculation of the elastic energy E_{el} [23] and defect energy ΔE [12, 20, 22] one gets that for a *fixed* pair the elastic energy E_{el} dominates the pinning energy E_{pin}, i.e. $\Delta E \sim E_{\mathrm{el}}$, and for the *completely optimized* pair the situation is vice versa, i.e. $\Delta E \sim E_{\mathrm{pin}}$. The resulting scaling behaviour is found to be $\Delta E \sim \ln(L)$ and $\Delta E \sim -\ln^{3/2}(L)$, respectively [12]. The scaling behaviour of the *fixed* dislocation pair in presence of pinning disorder is essentially equivalent to the one of a *fixed* defect pair at finite temperatures T without disorder, i.e. $\Delta E \sim \ln(L) \sim E_{\mathrm{el}}^{\mathrm{pure}}(T)$.

The density ρ of defects can be related to the length scale ξ_D beyond which the dislocations become unpaired [20] since for $\alpha \approx 0.6$ the density ρ, equation (9), shows the same scaling behaviour as ξ_D in the case of low temperatures and large core energy E_{c}, i.e. $E_{\mathrm{c}} \gg K \ln(\xi_D)$. For $E_{\mathrm{c}} \approx 0$ we found large densities ρ and one is probably out of the regime given by $E_{\mathrm{c}} \gg K \ln(\xi_D)$. This would possibly explain the occurrence of the stretched exponential behaviour close to $E_{\mathrm{c}} \approx 0$ as seen in figure 6(*a*).

To summarize, we have studied the effect of dislocation pairs on the ground state properties of the SOS model on a disordered substrate. For a fixed position of the dislocation pair a distance L apart we found that on average the defect *costs* an energy proportional to $\ln L$, in agreement with the findings for the energy costs for a steplike excitation step with fixed endpoints reported earlier [7] and also in agreement with recent results for other two-dimensional lattice models [12, 14]. On the other hand, if we optimize the position of the dislocation pair we showed that it *gains* energy, namely an amount proportional to $\ln^{\psi} L$ with an exponent ψ around $\frac{3}{2}$ as predicted by scaling arguments and also observed in the FPL model [12]. When introducing a penalty for the topological defects (i.e. a core energy) we showed that the density of defects vanishes exponentially as a function of this core energy, which is in agreement with the results for the FPL model [14]. Finally, we also demonstrated that a dislocation pair is screened by the presence of other dislocations in the system.

References

[1] Toner J and DiVincenzo D P 1990 *Phys. Rev.* B **41** 632
[2] Scheidel S 1995 *Phys. Rev. Lett.* **75** 4760
[3] Tsai Y-C and Shapir Y 1992 *Phys. Rev. Lett.* **69** 1773
Tsai Y-C and Shapir Y 1994 *Phys. Rev.* B **50** 3546

[4] Lancaster D J and Ruiz-Lorenzo J J 1995 *Phys.* A **28** 577 and references therein
[5] Zeng C, Middleton A A and Shapir S 1996 *Phys. Rev. Lett.* **77** 3204
[6] Blasum U, Hochstättler W, Moll C and Rieger H 1996 *J. Phys. A: Math. Gen.* 29 L459
[7] Rieger H and Blasum U 1997 *Phys. Rev.* B **55** 7394
[8] Rieger H 1998 Ground state properties of frustrated systems *Advances in Computer Simulation (Lecture Notes in Physics vol 501)* ed J Kertesz and I Kondor (Berlin: Springer)
[9] Alava M, Duxbury P, Moukarzel C and Rieger H 2000 Combinatorial optimization and disordered systems *Phase Transition and Critical Phenomena* ed C Domb and J L Lebowitz (New York: Academic) at press
[10] Chaikin P M and Lubensky T C 1997 *Principles of Condensed Matter Physics* (Cambridge: Cambridge University Press)
[11] Cieplak M, Maritan A and Banavar J 1994 *Phys. Rev. Lett.* **72** 2320
Porto M, Havli S, Schwarzer S and Bunde A 1997 *Phys. Rev. Lett.* **79** 4060
[12] Zeng C, Leath P L and Fisher D S 1999 *Phys. Rev. Lett.* **82** 1935
[13] Zeng C and Leath P L 1999 *Comput. Phys. Commun.* **121–122** 531
(Zeng C and Leath P L 1998 *Preprint* cond-mat/9810154)
[14] Middleton A A 1998 *Preprint* cond-mat/9807374
[15] Blatter G *et al* 1994 *Rev. Mod. Phys.* **66** 1125
[16] Giamarchi T and Le Doussal P 1998 *Statics and Dynamics of Disordered Elastic Systems* ed A P Young (Singapore: World Scientific) p 321
(Giamarchi T and Le Doussal P 1997 *Preprint* cond-mat/9705096)
[17] Nattermann T and Scheidl S 2000 On vortex-glass phases in impure superconductors *Adv. Phys.* at press
(Nattermann T and Scheidl S 2000 *Preprint* cond-mat/0003052
[18] Grüner G 1988 *Rev. Mod. Phys.* **60** 1129
[19] Li C C *et al* 1998 *Phys. Rev. Lett.* **60** 2765
[20] Le Doussal P and Giamarchi T 1998 *Preprint* cond-mat/9810218
[21] Rieger H 1998 *Phys. Rev. Lett.* **81** 4488
[22] Fisher D S 1997 *Phys. Rev. Lett.* **78** 1964
[23] Kosterlitz J M 1974 *J. Phys. C: Solid State Phys.* **7** 1046