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LETTER TO THE EDITOR

Self-duality in solid-on-solid models

H J F Knops

Instituut voor Theoretische Fysica, Katholieke Universiteit Nijmegen, Toernooiveld, 6525 ED Nijmegen, The Netherlands

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Abstract. It is shown that solid-on-solid models for which steps between neighbouring sites are limited to at most n adatoms exhibit self-dual points. At these points the amplitude of the height-height correlation function is exactly known. This extends a recent result of den Nijs for the case $n=1$. Some doubts are raised to his assertion that correction to scaling terms due to the sine-Gordon operators should be absent at self-dual points.

The solid-on-solid (SOS) model is well established as a model for crystal surfaces under equilibrium growth conditions. The Kosterlitz-Thouless transition that occurs in the SOS model corresponds to the roughening transition of the crystal surface (for a review see Weeks 1980). At temperatures above the roughening transition the height-height correlation function diverges logarithmically as

$$\langle (h_0 - h_r)^2 \rangle \simeq (\pi K)^{-1} \ln r. \tag{1}$$

The parameter K can be seen as the renormalised interaction strength of an effective Gaussian interaction (Kosterlitz and Thouless 1973, José *et al* 1977).

In general the SOS model is related under duality with the XY model (Knops 1977). It is the purpose of this letter to show that for special values of the interaction potential the SOS model is in fact self-dual. At these points the value of the renormalised coupling strength K is known exactly. It is useful to consider the duality between the SOS and XY models as a particular consequence of the duality relation for a more general model in which both vortices (with vorticity q) and sine-Gordon operators (favouring integral values) are present with fugacity y (respectively z). The partition sum of this model is defined by

$$Z_q(V, y, z) = \int_0^q \prod_i \mathrm{d}x_i \sum_{\{m_{\langle i,j\rangle}\}} \sum_{\{N_i\}} \exp\left(\sum_{\langle i,j \rangle} V(x_i - x_j + m_{\langle i,j\rangle} q) \right) \times \prod_i z^{N_i^2} \exp(2\pi \mathrm{i} x_i N_i) \prod_{i'} y^{M_{i'}^2}. \tag{2}$$

Here $\langle i, j \rangle$ denotes nearest-neighbour pairs on a square lattice and $M_i \equiv \sum m_{\langle i,j\rangle}$ where the sum is taken over the four nearest-neighbour pairs surrounding the site i' of the dual lattice. The duality relation for this model is (José *et al* 1977, Knops 1980)

$$Z_q(V, y, z) = Z_q(\tilde{V}, z, y) \tag{3}$$

with

$$\exp \tilde{V}(k) = q^{-1/2} \int_{-\infty}^{\infty} \mathrm{d}h \exp[V(h) + \mathrm{i}hk2\pi/q]. \tag{4}$$

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Both the SOS model and the XY model occur as special cases of $Z_q(V, y, z)$. The SOS model is obtained by setting $z=1$, which forces x_i to take integer values, and $y=0$, which excludes vortices. The XY model corresponds to the opposite case of a continuous model ($z=0$) having vortices with vorticity $q=2\pi$ and fugacity $y=1$. The XY interaction is given by the periodic continuation PV of V defined (for general q) by

$$\exp[PV(x)] = \sum_m \exp[V(x+qm)]. \tag{5}$$

The duality relation between the SOS model and the XY model is then a direct consequence of (3):

$$Z_{\mathrm{SOS}}(V) = Z_{2\pi}(V, 0, 1) = Z_{2\pi}(\tilde{V}, 1, 0) = Z_{XY}(P\tilde{V}). \tag{6}$$

As it is clear that the role of vortices and sine-Gordon operators are interchanged under duality it would seem that only models with $y=z$ can be self-dual. Indeed q-state clock models defined by

$$Z_{q\text{-CL}}(PV) = Z_q(V, 1, 1) \tag{7}$$

are known to be self-dual. However, this is not the only possibility since for a special choice of the interaction V the fugacity y becomes redundant and the self-duality may extend to $y=0$, i.e. the SOS models. In the particular case $q=5$ this has recently been noticed by den Nijs (1985a, b). Here the general case, which turns out to be $q=4n+1$, is considered.

The basic idea is to construct a potential that leads to a diverging core energy for the vortices. On a square lattice this is simply achieved by the requirement

$$\exp V(h) = 0 \qquad \text{for } |h| > n. \tag{8}$$

This choice limits steps between neighbouring sites to values $0, \pm 1, \ldots, \pm n \pmod q$. Since the core of a vortex on a square lattice consists of four such steps, one concludes that a vortex of vorticity $q=4n+1$ cannot occur. The value of the vortex fugacity is immaterial and may as well be set equal to zero. Consequently one has for a potential that satisfies (8)

$$Z_{q\text{-CL}}(PV) = Z_q(V, 1, 1) = Z_q(V, 0, 1) = Z_{\mathrm{SOS}}(V) \tag{9}$$

and the duality relation now reads

$$Z_{\mathrm{SOS}}(V) = Z_{q\text{-CL}}(P\tilde{V}). \tag{10}$$

Here $P\tilde{V}$ is found by combining (4) and (5) as

$$\exp[P\tilde{V}(k)] = q^{-1/2} \sum_{h=1}^{q} \exp[PV(h) + \mathrm{i}hk2\pi/q]. \tag{11}$$

The SOS model is self-dual when $\exp(P\tilde{V}) = \lambda \exp(PV)$ at the integer values $k=1, \ldots, q$. At first sight this seems hard to achieve in view of the requirement (8) which leaves only $2n+1$ Boltzmann weights free to satisfy $q=4n+1$ equalities. However, it is easy to see that, due to the fact that (11) is a Fourier sum, it suffices to demand that $\exp(P\tilde{V})$ satisfies (8). This involves only $2n$ equations that can therefore be solved to yield (up to a factor) a unique solution $\exp(PV^*)$. This solution is in fact self-dual. If it were not, $\exp(P\tilde{V}^*)$ would constitute a second solution since both $\exp(P\tilde{V}^*)$ and its dual $\exp(P\tilde{\tilde{V}}^*) = \exp(PV^*)$ satisfy (8). The Boltzmann weights of the self-dual SOS models that are found for $n=1, \ldots, 7$ are given in table 1. The case $n=1$ is the result of den

Table 1. Boltzmann weights $\exp PV^*(n)$ for self-dual SOS models. The exact value of the effective Gaussian coupling is shown in the left-hand column.

$K=\frac{2}{4n+1}$	$\lvert h\rvert=0$	1	2	3	4	5	6	7
$\frac{2}{3}\pi$	1	0.618	0	0	0	0	0	0
$\frac{2}{5}\pi$	1	0.742	0.258	0	0	0	0	0
$\frac{2}{13}\pi$	1	0.806	0.401	0.097	0	0	0	0
$\frac{2}{17}\pi$	1	0.844	0.497	0.187	0.034	0	0	0
$\frac{2}{21}\pi$	1	0.870	0.566	0.264	0.080	0.012	0	0
$\frac{2}{25}\pi$	1	0.889	0.619	0.329	0.127	0.032	0.004	0
$\frac{2}{29}\pi$	1	0.902	0.660	0.385	0.174	0.058	0.013	0.001

Nijs (1985b). As noticed in this reference the self-dual points in the SOS model have the interesting property that the value of the effective Gaussian coupling K is exactly known at these points. The reason is that under duality, sine-Gordon operators are mapped onto vortices with vorticity $q=4n+1$. The scaling indices of both operators can be expressed in the effective Gaussian coupling as $X_{SG}=\pi/K$ (respectively $X_q=Kq^2/4\pi$) (Kadanoff 1979). At the self-dual point these indices must be equal which implies $K_n=2\pi/(4n+1)$. Strictly speaking this conclusion is only valid provided the model is known to be in its rough phase. There is however no doubt that this is indeed the case because all the SOS models in table 1 represent surfaces that are substantially weaker than the roughening point of the restricted (i.e. $\exp[V(h)]=0$, $|h|>1$) SOS model estimated at $\exp[V(1)]\simeq 0.53$ (Luck 1981). Moreover this conclusion is consistent with the fact that the predicted Gaussian couplings K_n are located below the roughening value $K_r=\frac{1}{2}\pi$.

The self-dual SOS models decrease in coupling strength as n increases (see table 1). For $n>5$ these models are well represented by the Gaussian form

$$\exp[PV^*(h)]\simeq\exp(-\tfrac{1}{2}K_nh^2) \tag{12}$$

with an overall deviation of about 1%. On the one hand this fact can be understood from the way in which PV^* is constructed: in the continuum limit the Gaussian form (12) is the function with fastest decay that leaves (11) invariant. On the other hand it is also consistent with the renormalisation picture according to which in the high temperature limit Gaussian couplings in the SOS model remain almost constant while the sine-Gordon fugacity z is renormalised to zero (José *et al* 1977).

I am not convinced by the arguments given by den Nijs (1985b) that the effective value of the sine-Gordon fugacity z should already be zero for self-dual SOS models. He argues as follows: an SOS model that satisfies (8) may be seen as a clock model for which the vortices are effectively forbidden ($y=0$); under duality vortices are mapped onto sine-Gordon operators so that after duality $z=0$. As the model is self-dual both y and z should be equal to zero. The error in this reasoning is that the model is only self-dual provided it is discrete both before and after duality. This is clear since PV^* is left invariant by (11) only for discrete values of the argument k. Phrased more formally one does have, using the redundancy of the vortex fugacity (respectively duality),

$$Z_q(V^*,0,1)=Z_q(V^*,y,1)=Z_q(\tilde{V}^*,1,y) \tag{13}$$

for general y. However one may continue to write

$$Z_q(\tilde{V}^*, 1, y) = Z_q(V^*, 1, y) = Z_q(V^*, 0, y) \tag{14}$$

just in case $y = 1$ since $\tilde{V}^* = V^*$ at integer values only. The conclusion $Z_q(V^*, 0, 1) = Z_q(V^*, 0, 0)$ is therefore not justified. This means that a finite-size calculation should in principle show corrections to scaling both from the sine-Gordon operator and from the interaction shape. The fact that the former (which are asymptotically dominant) are not seen in the finite-size calculation for $q = 5$ (den Nijs 1985b) is probably due to the relatively small sizes (up to $L = 10$) considered. This belief is further strengthened by the fact that corrections to scaling from the sine-Gordon operator is also not found for potentials $V \neq V^*$.

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