Corrections to scaling and self-duality in the restricted solid-on-solid model

1985 J. Phys. A: Math. Gen. 18 L549

(http://iopscience.iop.org/0305-4470/18/9/011)

J. Phys. A: Math. Gen. **18** (1985) L549-L556. Printed in Great Britain

LETTER TO THE EDITOR

Corrections to scaling and self-duality in the restricted solid-on-solid model

Marcel den Nijs

Department of Physics, University of Washington, Seattle, Washington 98195, USA

Received 15 March 1985

Abstract. The corrections to scaling at and above the roughening transition T_R in the restricted solid-on-solid model are studied by means of finite-size scaling for semi-infinite strips of width 2 to 10. It is shown that at a temperature T_{SD} not far above the roughening temperature, where the restricted solid-on-solid model is invariant under the duality transformation of the five-state clock model, the fugacity of the sine-Gordon operator must vanish. For the dual truncated planar model this means that the core energy of the vortices diverges. Between T_S and T_R the corrections to scaling do not reach their asymptotic behaviour, but are dominated by the contributions from the $(\nabla\phi)^4$ operator associated with the restriction to steps of height one.

The properties of the vortex unbinding transition in the planar model, and of the roughening transition in solid-on-solid (SOS) models are well established. They are described by the Kosterlitz-Thouless (KT) theory (for a review on surface roughening see Weeks 1980). In SOS models interfaces and surfaces are characterised by integer valued column height variables h_r at the sites of a (square) lattice

$$Z_{\mathrm{RSOS}} = \sum_{\{h_r\}} \exp\Big(\sum_{\langle r,r' \rangle} J(1-(h_r - h_{r'})^2) \Big). \tag{1}$$

The restricted solid-on-solid (RSOS) model is the special version where only steps of height one are allowed, $h_r - h_{r'} = 0, \pm 1$. This restriction facilitates numerical studies (see e.g. Luck 1981) and seems justified in the context of experimental realisations such as the roughening of stepped metal surfaces like Ni (Conrad *et al* 1985) and Cu (Villain *et al* 1984). This restriction has also been applied in studies of the planar model. SOS models are equivalent to the planar model under duality transformations (Knops 1977). The RSOS model is dual to the so-called truncated planar model (Luther and Scalapino 1977) where the eigenstates of the angular momentum operator (in the transfer matrix) are restricted to the values 0 and ± 1. In the Hamiltonian limit the RSOS model is also equivalent to a spin-1 quantum chain (see e.g. Hamber and Richardson 1981, Botet and Jullien 1983, Solyom and Zimann 1984, den Nijs 1982).

The purpose of this paper is twofold. First it is pointed out that at one specific temperature J_{SD} the RSOS model is invariant under the duality transformation of the five-state clock model. This implies that the fugacity of the sine-Gordon (SG) operator (associated to the discreteness of the step heights) vanishes, i.e. that the core energy of the vortices in the truncated planar model diverges. The behaviour of the corrections to scaling in the finite size scaling calculation confirms this.

0305-4470/85/090549+08$02.25

Finite size scaling calculations have been applied to the RSOS model before (see above). They confirm the KT nature of the roughening transition, but compared to the very accurate results for e.g. Ising and Potts models, the convergence is poor. The second aim of this calculation is to determine whether a careful study of the corrections to scaling for the recently discovered universal amplitude in the scaling behaviour of the step free energy (Luck 1982, Nightingale and Blote 1983, Cardy 1984) improves the evidence for the KT nature of the transition, or whether there remains no other alternative than to increase the strip width by an order of magnitude. Strip width 10 is a natural upper limit for models with three states per site or per bond like the RSOS model, if the largest eigenvalues of the transfer matrix are obtained by multiplication while storing the entire wavefunction. It turns out that strip width $N = 10$ is already large enough such that the corrections to scaling are determined by the critical exponents and fugacities of the leading irrelevant scaling fields only. The two leading sources of corrections to scaling are the SG operator, associated with the discreteness of the step height (the vortex operator in the planar model), and the $(\nabla\phi)^4$ operator, associated with the restriction to steps of height one. Asymptotically the corrections to scaling must be dominated by the SG operator, but it turns out that for strip widths 2 to 10 the contribution from the $(\nabla\phi)^4$ operator dominates. This must be attributed to the step-1 restriction, and is enhanced by the vanishing of the SG fugacity at the self-dual point. The evidence of the KT nature of the transition improves with the understanding of the corrections to scaling, but to obtain a really good test of the KT theory the strip width must be increased by an order of magnitude or the RSOS must be modified such that the ratio between the fugacities of the SG and $(\nabla\phi)^4$ operator becomes more favourable.

It is useful to summarise the KT theory first. In the high-temperature rough phase the height fluctuations do not have a characteristic maximum cut-off. The height–height correlation function diverges logarithmically

$$\langle (h_{r+r_0} - h_{r_0})^2 \rangle \simeq (\pi K_G)^{-1} \log r, \qquad \text{when } r \gg 1. \tag{2}$$

The temperature dependent parameter K_G characterises the surface roughness. Since for those long wavelength fluctuations the discreteness of the column height variables is irrelevant, the rough surface can be described by the Gaussian model (Kosterlitz and Thouless 1973). Consider the following version of the sine-Gordon model (José *et al* 1977)

$$Z = \sum_{\{\{\phi_r, N_r\}\}} \exp\left[\sum_{\langle r,r' \rangle} -\tfrac{1}{2} K (\phi_r - \phi_{r'})^2 \right] \prod_r (z^{N_r^2} \exp[2\pi i \phi_r N_r]) \tag{3}$$

with $-\infty < \phi_r < \infty$ a continuous variable replacing h_r; $\exp(2\pi i \phi_r)$ the SG operator, favouring integer values; and $N_r = 0, \pm 1, \pm 2, \ldots$ an integer valued variable. In the limit of zero fugacity $z = 0$ this model reduces to the Gaussian model, for small z to the standard sine-Gordon model, and for $z = 1$ to the SOS model. The RSOS model is obtained by introducing additional weight functions $P(\phi_r - \phi_{r'})$: $P(x) = 0$ for $|x| > \frac{3}{2}$ and $P(x) = 1$ for $|x| < \frac{3}{2}$. $P(x)$ introduces corrections to the pure Gaussian interaction. The leading contribution is a $(\phi_r - \phi_{r'})^4$ interaction. The RT equations for the sine-Gordon model are known exactly for small fugacity

$$\mathrm{d}x/\mathrm{d}l = y^2, \qquad \mathrm{d}y/\mathrm{d}l = xy \tag{4}$$

with $x = 2 - \pi/K$ and $y = 4\pi z A$ (Kosterlitz 1974, José *et al* 1977, Amit *et al* 1980, Knops and den Ouden 1980). The high-temperature ($x < 0$) rough phase flows towards

the Gaussian model fixed line at $z = 0$. The fixed point value of the Gaussian coupling constant is equal to the surface roughness parameter K_G in equation (2). The roughening transition takes place at $K_G = \pi/2$, where the Gaussian fixed line becomes unstable with respect to the SG operator. The weight function $P(x)$ does not change these results, because the interactions it introduces are irrelevant at the Gaussian fixed line; the critical exponent of the $(\nabla\phi)^4$ operator is equal to $y_4 = -2$.

The fugacity parameter y in equations (4) includes both the bare fugacity z and the core energy $\log A$. The core energy takes into account the short distance deviations from the logarithmic interactions between vortices; A depends on the lattice cut-off and varies with temperature. At the roughening transition in the planar and unrestricted SOS model y is equal to $y_R = 0.495$ (Kosterlitz 1974, José *et al* 1977). In the RSOS model, as shown below, A vanishes at the self-dual temperature and increases to $y_R = 0.25 \pm 0.2$ at the roughening transition.

The duality of the RSOS model remains well hidden until one studies the RSOS model as a limit case of the five-state clock model (den Nijs 1985a). At one special temperature, $J_{SD} = \log[(\sqrt{5}+1)/2] = 0.4812$, the RSOS model is invariant under the duality transformation of the five-state clock model. This implies that at this special temperature the core energy A vanishes ($y = 0$), and yields the exact value of the roughness parameter, $K_G = \frac{2}{5}\pi$ ($x = -\frac{1}{2}$).

In analogy with equation (3), the five-state clock model can be visualised as a Gaussian model where in addition to the SG operator (to introduce discreteness in the steps) also vortices of Burgers' vector 5 (to introduce the periodicity after five clockwise steps) are included (José *et al* 1977). In the limit where the states $dh = \pm 2$ are frozen out the five-state clock model reduces to the RSOS model.

The duality equations for clock models are well known (José *et al* 1977, Elitzur *et al* 1979) and need not be repeated here. Also the connection between the RSOS model and the five-state clock model has been explained elsewhere (see, e.g., den Nijs 1985a). It is a direct consequence of the general structure of duality transformations that at the self-dual point in the RSOS model y vanishes. The duality transformation maps the five-state clock model into itself. It maps high temperatures onto low temperatures and maps the vortex operator onto the SG operator. It is a surprise to find a self-dual point in the RSOS model because this model lacks vortices, while under duality its SG excitations transform into vortices. Indeed in general the RSOS model maps onto another line in the five-state clock model. This line intersects with the RSOS model at one isolated self-dual point J_{SD}. To be consistent the SG excitations must be absent in the RSOS model at J_{SD}.

In the limit where the five-state clock model reduces to the RSOS model the vortices are frozen out in an indirect way. The core energy diverges due to a conspiracy between the step energies (step heights ± 2 become forbidden) and the coordination number of the square lattice (there is no way to make a vortex of Burgers' vector 5 without step sizes ± 2 at the four bonds emerging from each vertex). Similarly the bare fugacity z in (3) does not vanish. It is the core energy $\log A$ which diverges (see (4)); the SG operator is redundant at the self-dual point due to a hidden symmetry.

The roughness parameter is equal to $K_G = \frac{2}{5}\pi (x = -\frac{1}{2})$, because at J_{SD} the critical exponent of the vortex and SG operator must be equal (José *et al* 1977).

The finite size scaling behaviour of the step free energy in semi-infinite strips of width $N \leqslant 10$ confirms the redundancy of discreteness of the steps at J_{SD}. As usual the step free energy is obtained by comparing the largest eigenvalues of the transfer matrix, for different boundary conditions at the strip edge, $h_{N,y} = h_{0,y} + m$ (for reviews

see Nightingale (1982) and Barber (1983)). Above the roughening temperature $J < J_R$ the step free energy goes to zero as $\eta_m = S_m/N$. The amplitude S_m is a universal function proportional to the surface roughness parameter $S_m = \frac{1}{2}K_G m^2$ (Luck 1982). For the Gaussian model (the fixed line) this follows trivially by restoring the periodic boundary conditions via the transformation $\tilde{\phi}_{x,y} = \phi_{x,y} - mx/N$.

Figure 1 shows the finite size scaling behaviour of S_1. $J = 0$ corresponds to infinite temperature, the self-dual point is located at $J_{SD} = 0.4812$, and the roughening transition at $J_R = 0.63$. The antiferromagnetic RSOS model ($J < 0$) describes a surface, above its roughening transition, with loop-like internal degrees of freedom; the transition at $J_S = -0.4815$ belongs to same universality class as an Ising model on a lattice with transverse vibrations (den Nijs 1985b).

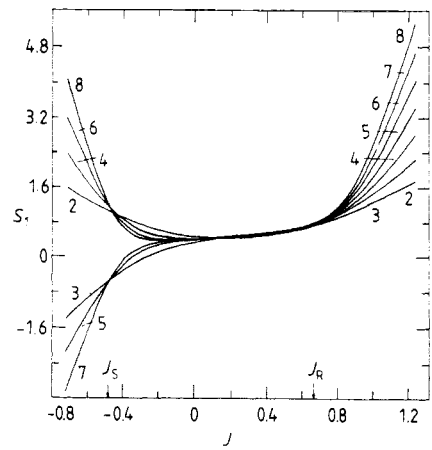

Figure 1. The step free energy times the strip width N of the RSOS model for $N = 2$ to 8.

At the roughening temperature the roughness parameter K_G has the universal value $\frac{1}{2}\pi$ (see (4)). J_R can be estimated from the sequence of temperatures where $S_1(N) = \frac{1}{2}K_G = \frac{1}{4}\pi$, see figure 2. At first sight the convergence looks very good. The approximants seem to converge linearly in $1/N$ to the value $J_R = 0.644 \pm 0.002$. However, according to the KT theory the convergence should be logarithmic (as discussed below). The asymptotic behaviour has not yet been reached. This is also more directly visible in figure 1; the KT theory predicts a square root singularity $(J - J_R)^{1/2}$ in the roughness parameter $K_G = 2S_1$ at J_R. This singularity is not yet established for strip widths $N \leqslant 10$.

The KT nature of a phase transition is usually tested by the behaviour of the Roomany-Wyld (RW) approximants for the beta function at the low-temperature side of the roughening transition

$$\beta_{RW}(N', N) = \frac{\log(S'/S)}{\log(N'/N)}\left[\frac{S'S}{(dS'/dJ)dS/dJ}\right]^{1/2}. \tag{5}$$

The KT theory predicts an essential singularity in the correlation length

$$\xi^{-1} \sim \eta \sim \exp(-b|J - J_R|^{-\sigma}) \tag{6}$$

with an exponent $\sigma = \frac{1}{2}$. The beta function is proportional to the first derivative of the

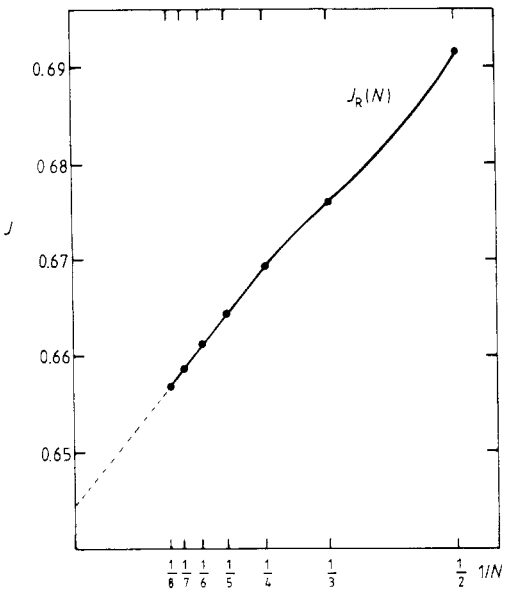

Figure 2. Approximants for the roughening temperature from the universal value of the amplitude of the step free energy.

logarithm of the correlation length with respect to temperature (see Barber 1983 for a review).

$$\beta_{\mathrm{RW}} = \frac{1}{\sigma b}|J - J_{\mathrm{R}}|^{1+\sigma}. \tag{7}$$

The RW approximants are shown in figure 3. As usual estimates for the parameters are not very accurate: $b = 2.2 \pm 0.1$, $\sigma = 0.50 \pm 0.05$, and $J_{\mathrm{R}} = 0.64 \pm 0.03$. The prefactor b contains information about the fugacity y_{R} at the roughening transition. The difficulty is that b not only depends on y_{R}, but also on the slope $\mathrm{d}y/\mathrm{d}x$ at J_{R} of the (effective)

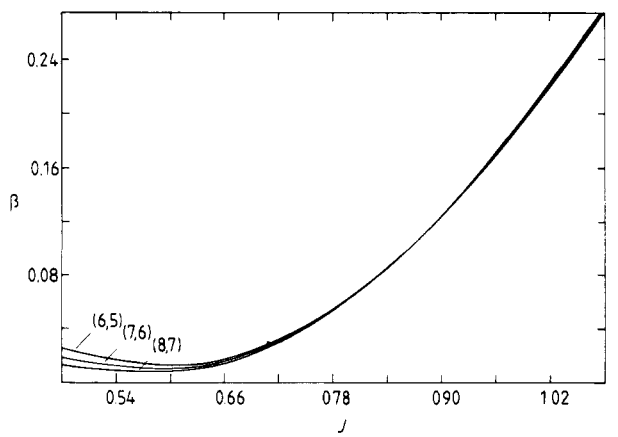

Figure 3. Roomany-Wyld approximants for the beta function $\beta_{\mathrm{RW}} = (N', N)$.

path that the RSOS model follows through the (x, y) phase diagram, and on the difference between the temperature variables K and J in the sine-Gordon and RSOS model,

$$\pi^3 = 2b^2(1+\mathrm{d}y/\mathrm{d}x)(\mathrm{d}K/\mathrm{d}J)y_R(2+y_R^2). \tag{8}$$

The slope can be approximated by $\mathrm{d}y/\mathrm{d}x = y_R/(1/2-y_R)$. $\mathrm{d}J/\mathrm{d}K$ can be estimated from the slope of $S_1(J) = \frac{1}{2}K_G(J)$ in figure 1 at high temperatures $J \ll J_R$, because in the sine-Gordon model the roughness parameter K_G becomes equal to the bare coupling constant K for $y \ll x < 0$. $\mathrm{d}S_1/\mathrm{d}J = 0.28$ at infinite temperature $J = 0$ and increases to $\mathrm{d}S_1/\mathrm{d}J = 0.56$ at the self-dual point $J = 0.4812$, so $\mathrm{d}J/\mathrm{d}K$ is of order 1. This leads to an order of magnitude estimate of $y_R \simeq 0.25$. This value is comparable to the one in the unrestricted SOS model $y_R = 0.4951$ (quoted above). This estimate is also consistent with the vanishing of y at the self-dual point; between J_{SD} (in the effective phase diagram (x, y) located at $(x, y) = (-\frac{1}{2}, 0)$) and J_R (the line $y = -x$) one would expect that y grows to a value $0.1 < y_R < 0.4$.

Figure 4 shows the corrections to scaling of the amplitude S_1 above the roughening temperature. In the Gaussian model itself there are no finite size corrections to the relation $S_m = \frac{1}{2}K_G m^2$. The RSOS model contains two leading corrections to scaling:

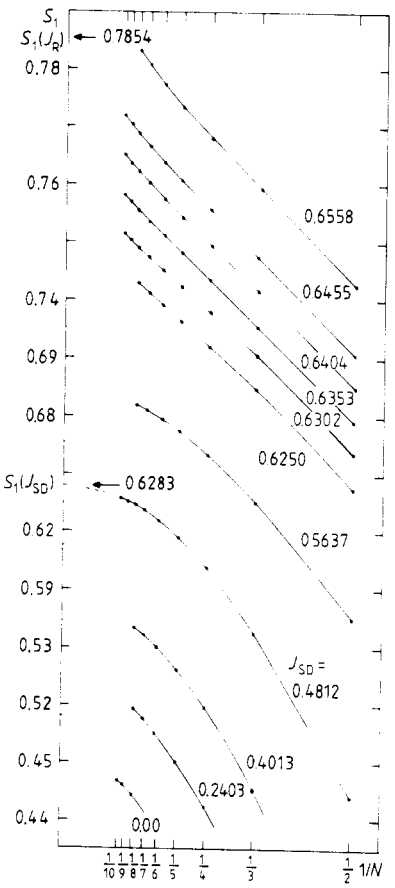

Figure 4. Correction to scaling behaviour of the amplitude of the step free energy for several temperatures J.

from the SG operator, and from the $(\nabla\phi)^4$ operator. Asymptotically the SG exponent should dominate, because its critical exponent $y_{SG}=2-\pi/K_G$ is larger than the exponent $y_4=-2$ of the $(\nabla\phi)^4$ operator

$$S_1=\tfrac{1}{2}K_G+CyN^{(2-\pi/K_G)}+LN^{-2}+\ldots. \tag{9}$$

Besides these, also contributions from all multiples and linear combinations of these two irrelevant critical exponents are present. At the self-dual point where $y=0$ only the corrections to scaling from the $(\nabla\phi)^4$ operator should remain

$$S_1=\tfrac{1}{2}K_G+LN^{-2}+\ldots. \tag{10}$$

Figure 4 confirms this. At $J_{SD}=\log[(\sqrt{5}+1)/2]=0.4812$, S_1 converges with a $1/N^2$ power instead of the $N^{-1/2}$ power predicted from (9). The amplitude is equal to $L=-0.233\pm0.003$. The extrapolated value $S_1=0.628\,318\pm0.000\,001$ is so close to the exact value $S_1=\frac{1}{2}K_G=\frac{1}{5}\pi$ that it is justified to conclude that indeed y is equal to zero. Moreover this rate of convergence confirms that strip width $N=10$ is sufficient to reach the scaling region where the corrections to scaling are dominated by the leading irrelevant scaling fields.

The $1/N^2$ power also fits $S_1(N)$ at all other temperatures except those very close to the roughening transition; asymptotically, the curves should have a cusp (the exponent $2-\pi/K_G$ is larger than -1 for all $J>0.24$). The conclusion must be that the fugacity y remains too small compared to the coupling constant L; for strip widths $N\leqslant 10$ the corrections to scaling due to the discreteness of the steps are swamped by those due to the step-1 restriction. This is consistent with the estimate $y<y_R\simeq 0.25$ from the beta function, and the value $L=-0.233$ at J_{SD}.

At the roughening transition the SG operator becomes marginal and S_1 must behave as

$$S_1=\tfrac{1}{4}\pi+C\frac{y}{1+y\log N}+LN^{-2}+\ldots. \tag{11}$$

Ideally the roughening transition should be determined by a fit of the $S_1(N)$ curves in the $0.625<J<0.645$ interval to this behaviour. From figure 4 it is clear that this can not be done satisfactorily. The SG contribution does not show its full structure until $N>\exp(1/y_R)\simeq 50$. Notice that someone unaware of this is likely to fit the data to a polynomial in $1/N$, and is led to believe that J_R is equal to $J_R=0.645$ (consistent with the $1/N$ extrapolation in figure 2) with an erroneously small error bar. All the curves close to J_R can be fitted to (11) with an average deviation less than 0.002 (twice the diameter of the dots in figure 4) using a least squares fit which optimises C and y for fixed values of L. However if y and L are restricted to the intervals $y=0.25\pm0.2$ and $L=-0.11\pm0.01$, the roughening transition narrows down to the interval $J_R=0.633\pm0.003$. The average deviation of the fit becomes less than 0.001, and $C=-0.050\pm0.006$. The value for L is obtained by extrapolation from around the self-dual point, $L(J)\simeq -0.233+0.78(J-J_{SD})$.

A closing comment on the five-state clock model phase diagram. A crucial aspect in the discussion of the string melting transition in the antiferromagnetic five-state clock model (den Nijs 1985a) was that the antiferromagnetic and ferromagnetic floating phases do not connect. The present calculation confirms this and improves the estimates for the end points of the two melting lines in the RSOS model. The string melting line ends at $J=-0.4815$ (see figure 1 and den Nijs 1985a). The melting line of the

ferromagnetic intermediate floating phase ends at the point where the roughness parameter is equal to $K_G = \frac{8}{25}\pi = 1.005$ (José *et al* 1977). Figure 4 shows that $J = 0.23$ is the endpoint.

This research is supported by the National Science Foundation under Grant No DMR 83-19301.

References

Amit D J, Goldschmidt Y Y and Grinstein G 1980 *J. Phys. A: Math. Gen.* **13** 585
Barber M 1983 in *Phase Transitions and Critical Phenomena* vol 8, ed C Domb and J L Lebowitz (New York: Academic)
Botet R and Jullien R 1983 *Phys. Rev.* B **27** 613
Cardy J 1984 *J. Phys. A: Math. Gen.* **17** L385, L961
Conrad E, Engel T, Riedel E and den Nijs M 1985 to be published
den Nijs M P M 1982 *Physica* **111A** 273
—— 1985a *Phys. Rev.* B **31** 266
—— 1985b *Preprint* University of Washington
Elitzur S, Pearson R and Shigemitsu J 1979 *Phys. Rev.* D **19** 3698
Hamber H W and Richardson J L 1981 *Phys. Rev.* B **23** 4698
José J V, Kadanoff L P, Kirkpatrick S and Nelson D 1977 *Phys. Rev.* B **16** 1217
Knops H J F 1977 *Phys. Rev. Lett.* **39** 766
Knops H J F and den Ouden L W J 1980 *Physica* **103A** 579
Kosterlitz J M 1974 *J. Phys. C: Solid State Phys.* 7 1046
Kosterlitz J M and Thouless D J 1973 *J. Phys. C: Solid State Phys.* **6** 1181
Luck J M 1981 *J. Physique Lett.* **42** 275
—— 1982 *J. Phys. A: Math. Gen.* **15** L169
Luther A and Scalapino D J 1977 *Phys. Rev.* B **16** 1153
Nightingale P 1982 *J. Appl. Phys.* **53** 7927
Nightingale P and Blote H 1983 *J. Phys. A: Math. Gen.* **16** L657
Solyom J and Zimann T A L 1984 *Preprint* CRIP, Budapest
Villain J, Grempel D R and Lapujoulade J 1985 *J. Phys. F: Met. Phys.* **15** 809
Weeks J D 1980 in *Ordering in Strongly Fluctuating Condensed Matter Systems* ed T Riste (New York: Plenum) p 293