Correlation functions in XY models and step free energies in roughening models

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A duality relation derived by José, Kadanoff, Kirkpatrick, and Nelson and by Knops is exploited to calculate properties of XY and roughening models from known properties of the dual models. It is shown that the correlation length in XY models is exactly given by $\xi^{-1}=\tilde{\beta}\tilde{f}$, where $\tilde{f}$ is the free energy per unit length of a step and $\tilde{\beta}$ is the inverse temperature in the corresponding roughening model. Similarly, the exponent η below T_c in an XY model is given by $\eta=\lim_{|\vec{r}|\to\infty}\tilde{\beta}\tilde{F}_1(\vec{r})/\ln|\vec{r}|$, where $\tilde{F}_1(\vec{r})$ is the free energy associated with two screw dislocations of unit strength and opposite sign separated by the distance $\vec{r}$ in the corresponding roughening model.

It has recently been demonstrated by José, Kadanoff, Kirkpatrick, and Nelson[1] (JKKN) and independently by Knops,[2] that a general two-dimensional XY model

$$H_{XY}=-\sum_{\langle fg\rangle}V(\phi_f-\phi_g)\ , \tag{1}$$

where $\pi\geq\phi_f>-\pi$ and the sum is over nearest neighbors, and a general two-dimensional roughening model

$$\tilde{H}=-\sum_{\langle fg\rangle}\tilde{V}(h_f-h_g)\ , \tag{2}$$

where h_f takes on all integral values, are dual to each other under the condition that

$$\exp[-\tilde{\beta}\tilde{V}(h)]=\frac{1}{2\pi}\int_{-\pi}^{\pi}d\phi\exp[-ih\phi-\beta V(\phi)]\ , \tag{3}$$

where β and $\tilde{\beta}$ are the respective inverse temperatures.

This interesting relationship provides a useful link between basic problems that have long been studied in the theories of magnetism and crystal growth. In this paper, we shall show one way in which this duality can be exploited to use results from the theory of crystal growth to obtain information about the XY model and vice versa.

In addition to the basic duality relation, JKKN[1] also showed that the XY-model correlation function

$$g_p(\vec{r}-\vec{r}')\equiv\langle\cos\{p[\phi(\vec{r})-\phi(\vec{r}')]\}\rangle \tag{4}$$

can be expressed for arbitrary p in terms of the roughening model as

$$g_p(\vec{r}-\vec{r}')=\tilde{Z}'/\tilde{Z}\ , \tag{5}$$

where

$$\tilde{Z}'=\sum_{\{h_f\}}\exp\left[-\tilde{\beta}\sum_{\langle fg\rangle}\tilde{V}(h_f-h_g-pn_{fg})\right]\ , \tag{6}$$

with the integers n_{fg} being equal to unity for bonds along a line connecting the dual lattice points $\vec{r}$ and $\vec{r}'$ (for f to the left of the line and g to the right) and zero elsewhere. $\tilde{Z}$ is the usual partition function for the roughening model [$\tilde{Z}=\tilde{Z}'(p=0)$].

The physical situation described by the partition function $\tilde{Z}'$ for integer values of p is a very familiar one in the theory of crystal growth.[3,4] It is that of two screw dislocations having strength p and opposite sign, which intersect the surface of the crystal at $\vec{r}$ and $\vec{r}'$. At zero temperature ($\tilde{T}=\tilde{\beta}^{-1}=0$), this leads to a step of height p running between $\vec{r}$ and $\vec{r}'$. (The step is straight and unique only if $\vec{r}$ and $\vec{r}'$ have the same x or y coordinates. Otherwise, there are several equivalent states, which give rise to a nonzero contribution to the entropy.) The primary interest in this configuration in the theory of crystal growth is as a continuous source of steps, which bypasses the nucleation barrier below the roughening temperature and greatly enhances the growth rate.[3]

Since the free energy associated with this step $\tilde{F}_p(\vec{r}-\vec{r}')$ is by definition just the difference in free energies of the system with and without the two screw dislocations, we see from Eq. (5) that

$$g_p(\vec{r}-\vec{r}')=\exp[-\tilde{\beta}\tilde{F}_p(\vec{r}-\vec{r}')]\ . \tag{7}$$

This is our basic equation.

If $|\vec{r}-\vec{r}'|$ is large, the contributions from the ends of the step become relatively unimportant for sufficiently large $\tilde{\beta}$ and, neglecting smaller (possibly logarithmic) terms

$$\tilde{F}_p(\vec{r}-\vec{r}')\to|\vec{r}-\vec{r}'|\tilde{f}_p\ , \tag{8}$$

where $\tilde{f}_p$ is the free energy per unit length associated with an infinitely long step of height p. This implies that

$$g_p(\vec{r}-\vec{r}') \rightarrow \exp(-|\vec{r}-\vec{r}'|\xi_p^{-1}) \ , \tag{9}$$

where the correlation length in the XY model is exactly given by

$$\xi_p^{-1} = \tilde{\beta}\tilde{f}_p \ . \tag{10}$$

Note that Eq. (10) implies that the suggestion by Leamy and Gilmer[5] that $\tilde{f}_1$ goes to zero at the roughening temperature, $\tilde{T}_R$, is identical to the statement that the correlation length in the XY model diverges at T_c. Similarly, $\tilde{f}_1 = 0$ above $\tilde{T}_R$ is consistent with the XY model having a line of critical points for $T \leq T_c$.[6,9] Indeed, it is known that

$$g_p(\vec{r}-\vec{r}') \sim |\vec{r}-\vec{r}'|^{-\eta p} = |\vec{r}-\vec{r}'|^{-p^2/2\pi\beta V''(0)} \tag{11}$$

at sufficiently low temperatures,[6,7] so that for sufficiently high temperatures in the roughening model, $\tilde{F}_p(\vec{r}-\vec{r}')$ is given asymptotically by[6,7]

$$\tilde{\beta}\tilde{F}_p(\vec{r}-\vec{r}') \rightarrow \left[\frac{p^2}{2\pi\beta V''(0)}\right] \ln|\vec{r}-\vec{r}'| = \eta_p \ln|\vec{r}-\vec{r}'| \ , \tag{12}$$

which is a new result in the theory of crystal growth. This establishes a direct link between the exponent η and the asymptotic behavior of the free energy of a step.

The second derivative of the equivalent XY interaction is easily found from Eq. (3) to be

$$\beta V''(0) = \sum_{n=-\infty}^{\infty} n^2 \exp[-\tilde{\beta}\tilde{V}(n)] \Big/ \sum_{n=-\infty}^{\infty} \exp[-\tilde{\beta}\tilde{V}(n)] \tag{13}$$

For the physically important case of the solid-on-solid (SOS) model[3]

$$\tilde{\beta}\tilde{V}_{\rm SOS}(n) = \tilde{\beta}\tilde{\epsilon}|n| \ , \tag{14}$$

we can immediately evaluate

$$\beta V''_{\rm SOS}(0) = 2e^{-\tilde{\beta}\tilde{\epsilon}}(1-e^{-\tilde{\beta}\tilde{\epsilon}})^{-2} \ , \tag{15}$$

so that

$$\tilde{F}_{p,\rm SOS}(\vec{r}-\vec{r}') \rightarrow (p^2/4\pi\tilde{\beta})e^{\tilde{\beta}\tilde{\epsilon}}(1-e^{-\tilde{\beta}\tilde{\epsilon}})^2 \times \ln|\vec{r}-\vec{r}'| \tag{16}$$

for high temperatures ($\tilde{\beta}$ small) and large separations.

In deriving Eqs. (12) and (16) from Eq. (7), we have made use of the fact that the low-temperature properties of XY models are relatively easily calculated to obtain a result that is valid for the more difficult high-temperature region of a roughening model. By the same token, we can use Eq. (10) together with available results for the low-temperature region of roughening models to calculate correlation lengths in the high-temperature phase of XY models.

If we are sufficiently far below $\tilde{T}_R$, the calculation of $\tilde{f}_1$ for a roughening model is equivalent to the calculation of the interface free energy in a two-dimensional Ising model. Thus, from Onsager's[10] solution, we have for a step in the [10] direction

$$\tilde{\beta}\tilde{f}_1([10]) \approx \tilde{\beta}[\tilde{V}(1)-\tilde{V}(0)] - \ln\coth\{\tfrac{1}{2}\tilde{\beta}[\tilde{V}(1)-\tilde{V}(0)]\} \ ; \tag{17}$$

and from Fisher and Ferdinand,[11] we have

$$\tilde{\beta}\tilde{f}_1([11]) \approx \sqrt{2}\ln\sinh\{\tilde{\beta}[\tilde{V}(1)-\tilde{V}(0)]\} \tag{18}$$

for a step in the [11] direction.

An immediate result is that for any XY model

$$\lim_{\beta\rightarrow 0}\frac{\xi([10])}{\xi([11])} = \lim_{\beta\rightarrow\infty}\frac{\tilde{f}_1([11])}{\tilde{f}_1([10])} = \sqrt{2} \ . \tag{19}$$

Equations (10), (17), and (18) can be easily evaluated for specific models of interest. For the original XY model, with

$$V_0(\phi) = -J\cos\phi \ , \tag{20}$$

we have[2]

$$\tilde{\beta}\tilde{V}_0(n) = -\ln I_n(\beta J) \ , \tag{21}$$

where $I_n(\beta J)$ is the Bessel function of imaginary argument.[12] This gives (in units of the lattice constant) for $p=1$,

$$\xi_{[10]}^{-1} \approx -\ln[I_1(\beta J)/I\ (\beta J)] - \ln[I_0(\beta J)-I_1(\beta J)] + \ln[I_0(\beta J)-I_1(\beta J)] \tag{22}$$

and

$$\xi_{[11]}^{-1} \approx -\sqrt{2}\ln 2 + \sqrt{2}\ln\left[1-\left[\frac{I_1(\beta J)}{I_0(\beta J)}\right]^2\right] - \sqrt{2}\ln\left[\frac{I_1(\beta J)}{I_0(\beta J)}\right] \ . \tag{23}$$

Since $I_1(z)/I_0(z) \rightarrow \frac{1}{2}z$ for small z the correlation lengths for the original XY model vanish as $(\ln T)^{-1}$ for high temperature.

Similarly, the Villain model[13]

$$\beta V_v(\phi) = -\ln\sum_{n=-\infty}^{\infty}\exp[-\beta A(\phi-2\pi n)^2] \ , \tag{24}$$

which is dual to the discrete-Gaussian (DG) model[2]

$$\tilde{V}_v(n) = (4\beta A)^{-1}n^2 \ , \tag{25}$$

has the correlation lengths

$$\xi_{[10]}^{-1} = (4\beta A)^{-1} - \ln\coth(1/8\beta A) \tag{26}$$

and

$$\xi_{[11]}^{-1} = \sqrt{2}\ln\sinh(1/4\beta A) \quad . \tag{27}$$

Note that for the Villain model the correlation lengths vanish as T^{-1} in the limit of high temperatures.

The high temperature behaviors of the original XY model and the Villain model are identical if we choose A such that

$$A = -\{4\beta \ln[I_1(\beta J)/I_0(\beta J)]\}^{-1}$$
$$\approx -[4\beta \ln(\tfrac{1}{2}\beta J)]^{-1} \quad , \tag{28}$$

which is just what Villain suggested on the basis of equating the first Fourier components of the interactions.[13]

Equations (22), (23), (26), and (27) for the correlation lengths all refer to the case $p = 1$. For $p > 1$, the results depend on the form of the dual interaction $\tilde{V}(n)$—even in the limit of very high temperatures.

If

$$\tilde{V}(n+1) - \tilde{V}(n) \geq \tilde{V}(n) - \tilde{V}(n-1) \tag{29}$$

for $n \geq 1$, the free energy per unit length of a step of height p can be reduced by separating it into p steps of unit height. Therefore, if inequality (29) holds, we have

$$\tilde{f}_p = p\tilde{f}_1 \tag{30}$$

and, hence,

$$\xi_p = \xi_1/p \quad . \tag{31}$$

However, if inequality (29) is violated, the step will then stay together so that

$$\tilde{f}_p \leq p\tilde{f}_1 \tag{32}$$

and

$$\xi_p \geq \xi_1/p \quad . \tag{33}$$

Clearly, the SOS model [Eq. (14)] marks a boundary between these two types of behavior.

So far, we have used low-temperature expansions in both models to obtain properties of the dual models at very high temperatures. Calculations near the transition are notoriously difficult in both models, but there are some immediate possibilities for making further progress that we shall now explore.

One possibility for calculating correlation lengths closer to T_c would be to apply mean-field theory to the corresponding roughening model. The basic theory for the SOS model [Eq. (14)] has been set forward by Temkin[14] (although the necessary equations were derived much earlier by Hill[15]) and the corresponding theory for the discrete Gaussian model [Eq. (25)] has been presented by Kim and Thompson.[16] These theories suffer from the drawback that they fail to predict a roughening transition ($\tilde{T}_R^{\rm MF} = \infty$). This failure has been explained and a mean-field theory that does show a transition has been constructed,[17] but the value for $\tilde{T}_R$ is much too high and, as yet, no calculations of step properties have been made.

Step properties have been calculated for the SOS model within the Temkin approximation[18-21] and clearly show the system becoming isotropic at higher temperatures (which corresponds to ξ becoming isotropic near T_c) but because of the failure to predict a roughening transition, $\tilde{f}_1^{\rm MF}$ remains finite at all temperatures.

A straightforward way of obtaining information on the correlation functions is by Monte Carlo simulations of steps in the roughening models. Both $\tilde{F}_p(\vec{r}-\vec{r}')$ and $\tilde{f}_p$ can be calculated in this way and simulations for $\tilde{f}_1$ have already been performed for both the SOS and DG models.[22] Unfortunately, the statistical errors are too large to obtain $\tilde{f}_1$ close to $\tilde{T}_R$, but the results do indicate that Eqs. (17) and (18) should be good up to about $\frac{1}{2}\tilde{T}_R$.

Another effect that has been seen in Monte Carlo simulations is the rounding of growth spirals as the temperature is raised.[4] Although spiral growth is a dynamic process, the shape of the spiral is related to the shape of the critical nucleus, which in turn depends on the isotropy of the step-free energy.[3] This implies that the rounding of the growth spirals in the roughening models is directly related to the isotropy of the correlation lengths in the corresponding XY models, and spiral rounding should always be observed as $\tilde{T}_R$ is approached.

Finally, although no exact solutions are known for any roughening model of the type discussed in this paper, van Beijeren[23] has presented an exact solution of a "body-centered solid-on-solid" (BCSOS) model which may have the same critical properties. The step-free energy for this model goes to zero at $\tilde{T}_R$ as $\exp(-\tilde{\alpha}|\tilde{T}-\tilde{T}_R|^{-1/2})$. If the models we have discussed have the same critical behavior, the corresponding XY model correlation lengths would diverge as

$$\xi \sim \exp(+\alpha|T - T_c|^{-1/2}) \tag{34}$$

as T_c is approached from above. It is interesting to note that this is exactly what Kosterlitz[9] has predicted from a renormalization group treatment of the Coulomb gas representation of the XY model.[24]

Note added in proof. Since this paper was submitted, I have learned that a relation quite similar to Eq. (10) has been found for the two-dimensional Ising

model. The duality argument was given by A. E. Ferdinand [Ph.D. thesis (University of London, 1967), Chap. 11] and the result is contained in an article by M. E. Fisher [J. Phys. Soc. Jpn. Suppl. 26, 87 (1969). See also P. G. Watson, J. Phys. C 1, 575 (1968); in *Phase Transitions and Critical Phenomena,* edited by C. Domb and M. S. Green (Academic, London, 1972), Vol 2, p. 115. The Ising model duality argument has been recently rediscovered by R. K. P. Zia [Phys. Lett. (to be published)].

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[1]J. V. José, L. P. Kadanoff, S. Kirkpatrick, and D. R. Nelson, Phys. Rev. B 16, 1217 (1977).

[2]H. J. F. Knops, Phys. Rev. Lett. 39, 766 (1977).

[3]W. K. Burton, N. Cabrera, and F. C. Frank, Philos. Trans. R. Soc. Lond. 243, 299 (1951).

[4]R. H. Swendsen, P. J. Kortman, D. P. Landau, and H. Müller-Krumbhaar, J. Cryst. Growth 35, 73 (1976).

[5]H. J. Leamy and G. H. Gilmer, J. Cryst. Growth 24/25, 499 (1974).

[6]F. Wegner, Z. Phys. 206, 465 (1967).

[7]V. L. Berezinskii, Zh. Eksp. Teor. Fiz. 59, 907 (1970) [Sov. Phys.-JETP 32, 493 (1971)].

[8]J. M. Kosterlitz and D. J. Thouless, J. Phys. C 6, 1181 (1973).

[9]J. M. Kosterlitz, J. Phys. C 7, 1046 (1974).

[10]L. Onsager, Phys. Rev. 65, 117 (1944).

[11]M. E. Fisher and A. E. Ferdinand, Phys. Rev. Lett. 19, 169 (1967).

[12]M. Abramowitz and I. A. Stegun, *Handbood of Mathematical Functions* (Dover, New York, 1965), p. 376.

[13]J. Villain, J. Phys. (Paris) 36, 581 (1975).

[14]D. E. Temkin, in *Crystallization Processes,* edited by N. N. Sirota *et al.* (Consultants Bureau, New York, 1966).

[15]T. L. Hill, J. Chem. Phys. 15, 767 (1947).

[16]D. Kim and C. J. Thompson, J. Phys. A 9, 2097 (1976).

[17]R. H. Swendsen, Phys. Rev. B 15, 689 (1977).

[18]R. H. Swendsen, J. Cryst. Growth 36, 11 (1976). The low-temperature results for the [11] step given in this paper are not correct due to the use of the symmetry $\sigma_{n,m}=-\sigma_{2-n,1-m}$ instead of $\sigma_{n,m}=-\sigma_{2-n,-m}$. The mean-field entropy for the [11] step should have a $\tilde{T}=0$ value that is one-half the exact value (see Ref. 11). This does not affect the results at higher temperatures where the thermodynamic properties become isotropic. I would like to thank Dr. G. H. Gilmer for bringing this to my attention.

[19]D. E. Temkin, Kristallografiya 19, 467 (1974) [Sov. Phys. Crystallogr. 19, 291 (1974)].

[20]D. E. Temkin and V. V. Shevelev, Kristallografiya 21, 293 (1976) [Sov. Phys. Crystallogr. 21, 158 (1976)].

[21]D. E. Temkin and V. V. Shevelev, Kristallografiya 21, 1024 (1976) [Sov. Phys. Crystallogr. 21, 588 (1976)].

[22]R. H. Swendsen, Phys. Rev. B 15, 5421 (1977).

[23]H. van Beijeren, Phys. Rev. Lett. 38, 993 (1977).

[24]For the connection between the *XY* model and the Coulomb gas, see Refs. 8, 9, 13, and S. T. Chui and J. D. Weeks, Phys. Rev. B 14, 4978 (1976).