θ_0 to be determined with three pieces of data namely r, η, and the tilt angle ω. The tilt angle is indeed expected to be different from θ_0, and given by

$$\tan\omega = \langle|\tan\theta|\rangle\langle\cos\varphi\rangle , \quad (2)$$

as can be easily inferred from geometrical considerations.

Choosing $u = 64°$, with $r = 0.242$, $\eta = 0.24$, and $\omega = 28°$ (the values for 134.5°C) we have found the following solution: $\theta_0 = 31.2°$, $\langle\delta\theta^2\rangle^{1/2} = 22°$, $\langle\cos\varphi\rangle = 0.97$ corresponding to $\langle\Delta\varphi^2\rangle^{1/2} \approx 14°$. This corresponds to an average amplitude fluctuation of the axis of about 20°, a value which is fairly consistent with what was estimated from the NQES results.[5] The fact that η decreases while r remains practically constant when the temperature is increased in the H phase is easily accounted for by an increase of the azimuthal fluctuation amplitude. For 139°C, we have found $\langle\delta\theta^2\rangle^{1/2} \approx 22°$ and $\langle\cos\varphi\rangle \approx 0.94$ corresponding to $\langle\Delta\varphi^2\rangle^{1/2} \approx 20°$.

In conclusion, for the VI phase, the present NQR and NQES results are quite consistent with one another but both do not allow discrimination between the various models. Model C is favored from other considerations.[6] For the H phase, the NQR results are consistent either with a uniaxial model with weak orientational ordering, or with a model permitting uniform rotation around the long axis and fluctuation of this axis. In this case, the latter should be favored since it agrees with the NQES results while the former does not.[3-6]

Finally, concerning the smectic-C phase, since the situation is essentially the same as in the smectic-H phase, there is clearly no need to invoke any orientational order around the long axis to explain the corresponding NQR data.[1] This will be discussed in detail in a forthcoming paper.

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[1]J. Seliger, R. Osredkar, V. Žagar, and R. Blinc, Phys. Rev. Lett. 38, 411 (1977).

[2]R. J. Meyer and W. L. McMillan, Phys. Rev. A 9, 899 (1974).

[3]H. Hervet, F. Volino, A. J. Dianoux, and R. E. Lechner, J. Phys. (Paris), Lett. 35, L151 (1974).

[4]H. Hervet, F. Volino, A. J. Dianoux, and R. E. Lechner, Phys. Rev. Lett. 34, 451 (1975).

[5]F. Volino, A. J. Dianoux, and H. Hervet, J. Phys. (Paris), Colloq. 37, C3-55 (1976).

[6]A. J. Dianoux, H. Hervet, and F. Volino, J. Phys. (Paris) 38, 809 (1977).

[7]In fact, the EFG has both intramolecular and intermolecular origins. In a solid, the latter is usually found to contribute no more than 3 to 4% change in the quadrupole coupling constants [A. Coker, T. Lee, and T. P. Das, J. Chem. Phys. 66, 3903 (1977)]. The accuracy on $|eq_0|$ is thus expected to be of this magnitude while that on η_0 may be (much) poorer. These quantities can thus be also considered, to a certain extent, as parameters. For our present purpose, however, this is not necessary.

Exact Relation between the Solid-on-Solid Model and the XY Model

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An exact relation is established between the solid-on-solid model describing the growth of crystals and the classical XY model. Application of this relation to a special case leads to an exact correspondence between the XY model and the Coulomb gas which matches with the relation obtained by Kosterlitz in the strong-coupling limit.

Recently there has been a growing interest in the existence and nature of a roughening transition which might describe the sudden loss of a sharp interface in Monte Carlo simulations[1,2] of crystal growth. The interface in these simulations is described by the so-called solid-on-solid (SOS) model in which the possibility of "overhangs" above the interface are ruled out so that the interface is conveniently described in terms of integers h_j denoting the number of adatoms at the jth lattice position of the interface. The interaction, which will be assumed here to be of nearest-neighbor type, is expressed in terms of height differences of adjacent columns as

$$H = \sum_{\langle i,j\rangle} V(h_i - h_j) . \quad (1)$$

Originally[3,4] the possibility of a roughening

transition was argued on the basis of a comparison with the two-dimensional Ising model, but recently it was shown by Chui and Weeks[5] that in the special case of the discrete Gaussian (DG) model, where the function V is quadratic, an exact mapping could be made onto the Coulomb gas. The nature of the transition in the latter model is believed to be rather different from that of the Ising model. Renormalization-group calculations by Kosterlitz[6] suggest a specific heat which is not analytic but infinitely differentiable at T_c (infinite-order transition) while the susceptibility remains infinite for all $T < T_c$. A second indication that the roughening transition of the SOS model is not the Ising type came from the work of van Beyeren.[7] He showed that the so-called BCSOS (body-centered SOS) model, which can be seen as a next-nearest-neighbor version of (1) with a V that allows only unit height differences, can be translated into the ice model. The exact solution of the latter model shows again a specific heat with an infinite-order singularity.

In the present Letter I want to show that the general SOS model can be mapped into a third model with an expected infinite-order singularity, namely the two-dimensional XY model.[8] The existence of such a relation is not completely unexpected since Kosterlitz and Thouless[9] pointed out that the vortex configurations in the XY model interact as charged particles in a Coulomb gas which in its turn is connected with the DG version of the SOS model as mentioned above. The present result is new because it applies to a general V and because it yields, upon restriction to a quadratic V, a precise mathematical relation between the XY model and the Coulomb gas which can be compared with the physical identification of Kosterlitz and Thouless.

Consider for simplicity the Hamiltonian (1) on a square lattice of N sites. We associate to each nearest-neighbor bond a new variable

$$n_{\langle ij\rangle} = h_i - h_j, \tag{2}$$

where the sign is chosen such that the lattice point i has a smaller x (or y) coordinate than the point j. A description of the model in terms of these variables would increase the number of degrees of freedom by a factor of 2 so that one should take into account N constraints which can be expressed by demanding that for every elementary square

$$n_{\langle ij\rangle} + n_{\langle jk\rangle} - n_{\langle kl\rangle} - n_{\langle li\rangle} = 0, \tag{3}$$

where the sites i, j, k, and l are the corners of the square. This constraint can be written as

$$(2\pi)^{-1}\int_0^{2\pi} d\varphi_{j'} \exp i\varphi_{j'}(n_{\langle ij\rangle} + n_{\langle jk\rangle} - n_{\langle kl\rangle} - n_{\langle li\rangle}) = \delta_{n_{\langle ij\rangle}+n_{\langle jk\rangle}, n_{\langle kl\rangle}+n_{\langle li\rangle}}, \tag{4}$$

where the angle $\varphi_{j'}$ may be associated to the centers of squares (numbered by j') thereby forming again a square[10] lattice. The partition function $Z(V)$ of the SOS model defined as

$$Z(V) = \sum_{h_1,\ldots,h_N} \exp\Big[-\sum_{\langle i,j\rangle} V(h_i - h_j)\Big] \tag{5}$$

may be evaluated by summing over the new variables $n_{\langle ij\rangle}$ taking into account for every square j' a constraint of the form (4). Interchange of the sum over $n_{\langle ij\rangle}$ and the integration over $\varphi_{j'}$ leads to decoupled sums over the $n_{\langle ij\rangle}$ with the result

$$Z(V) = (2\pi)^{-N}\int_0^{2\pi} d\varphi_1 \cdots \int_0^{2\pi} d\varphi_N \exp\Big[-\sum_{\langle i',j'\rangle} \tilde{V}(\varphi_{i'} - \varphi_{j'})\Big] \tag{6}$$

in which the function V has a period 2π and is defined by

$$\tilde{V}(\varphi) = -\ln\{\textstyle\sum_n \exp[in\varphi - V(n)]\}. \tag{7}$$

Formula (6) expresses the partition function of the SOS model as a partition function of a generalized XY model where next to the usual interaction term $J\cos(\varphi_{i'} - \varphi_{j'})$ also appear higher harmonics. These higher harmonics are absent if one considers a special SOS model with V given by

$$V(n) = -\ln(2/\pi)^{1/2}\int_0^{\pi} e^{J\cos\varphi}\cos(\varphi n)\,d\varphi = -\ln(2\pi)^{1/2} I_n(J), \tag{8}$$

where I_n is the Bessel function of imaginary argument.

A SOS model which is often considered in the Monte Carlo simulations is the model where the func-

tion V is given by

$$V(n)=J|n|\,, \tag{9}$$

the interaction of the corresponding XY model is easily calculated to be

$$\tilde{V}(\varphi)=-\ln(\tanh J)+\ln\left(1-\frac{2e^{-J}}{1+e^{-2J}}\cos\varphi\right). \tag{10}$$

A general feature of the transformation, which is directly apparent from this formula, is that strong couplings are mapped into weak couplings and vice versa.

One can use the result of Chui and Weeks[5] to establish a precise relation between the XY model and the Coulomb gas defined by a Hamiltonian

$$H=-J_{\mathrm{Coul}}\Big\{\sum_{i,j}p_i p_j \ln(|i-j|)+(\tfrac{1}{2}\ln 8+\gamma)\textstyle\sum_i p_i^{\,2}\Big\}\,, \tag{11}$$

where p_i denotes the charge located at lattice site i and γ is Euler's constant. Chui and Weeks show that the partition function of the discrete Gaussian SOS model with V given by

$$V(n)=J_{\mathrm{DG}}n^2 \tag{12}$$

is directly related to the partition function of a Coulomb gas defined by (11) with

$$J_{\mathrm{Coul}}=\tfrac{1}{2}\pi/J_{\mathrm{DG}}\,. \tag{13}$$

Notice that in this transformation again strong couplings are mapped into weak couplings.

The DG model (12) can in its turn be related, via the present result, to an XY model with an interaction

$$\begin{aligned}\tilde{V}(\varphi)&=-\ln\textstyle\sum_n \exp(in\varphi-J_{\mathrm{DG}}n^2)\\&=-\ln\theta_3[\tfrac{1}{2}\varphi,\ \exp(-J_{\mathrm{DG}})]\,,\end{aligned} \tag{14}$$

where θ_3 is the Jacobi θ function. It is, therefore, this special XY model which is exactly related to the Coulomb gas when we put $J_{\mathrm{DG}}=\frac{1}{2}\pi/J_{\mathrm{Coul}}$.[11] In order to compare this relation with that of Kosterlitz and Thouless[9] we consider the strong-coupling limit for the XY model (i.e., $J_{\mathrm{DG}}\to 0$) in which limit their result is expected to apply.

In that limit it is a good approximation to consider only the second-order term in the expansion of $V(\varphi)$ yielding

$$\tilde{V}(\varphi)=-\tfrac{1}{2}K(J_{\mathrm{DG}})\varphi^2, \tag{15}$$

where the function $K(J)$ is given asymptotically by

$$K(J_{\mathrm{DG}})=\tfrac{1}{2}J_{\mathrm{DG}}^{-1}+\cdots. \tag{16}$$

Comparison with the same expansion for the usual XY model leads in the strong-coupling limit to the relation

$$J_{XY}=\tfrac{1}{2}1/J_{\mathrm{DG}}=\pi^{-1}J_{\mathrm{Coul}}, \tag{17}$$

which corresponds exactly[12] with the result of Kosterlitz and Thouless. The estimate of the critical temperature of the XY model given by Kosterlitz[6] leads to the value $J_{\mathrm{DG}}^{-1}\simeq 1.48$ for the roughening temperature of the DG model. This value compares favorably with the value $J_{\mathrm{DG}}^{-1}\simeq 1.3\pm 0.1$ found in Monte Carlo simulations[2] of the DG model.

An important correlation function in the study of the roughening transition is

$$g(j)=\langle(h_0-h_j)^2\rangle, \tag{18}$$

which describes the average interface width between sites which are a distance $|j|$ apart. If one passes to the Fourier transform of the interface profile, the methods used above to transform the partition function are directly applicable and one finds

$$g(j)=[(d^2/d^2\theta)P(\theta;j)]_{\theta=0}. \tag{19}$$

The function $P(\theta;j)$ is defined by

$$P(\theta;j)=\frac{1}{Z(V)}\int_0^{2\pi}d\varphi_1\cdots\int_0^{2\pi}d\varphi_N\exp\Big[-\sum_{<i',j'>\in L^{\perp}}\tilde{V}(\varphi_{i'}-\varphi_{j'})-\sum_{<i',j'>\in L}\tilde{V}(\varphi_{i'}-\varphi_{j'}+\theta)\Big], \tag{20}$$

in which L denotes the set of bonds (on the dual XY lattice) which are crossed by a path S on the original lattice connecting the points 0 and j, and $L^{\perp}$ is the complement of L. This form of representing the correlation function $g(j)$ in terms of averages in the XY model has the advantage that it brings out clearly the independence on the choice of the path S, since the set L can be moved to the set L' corre-

sponding to another path S' by a shift over θ of all angles located between S and S'. Otherwise it is unfortunately a rather complicated expression. In order to get some insight into its structure, one may expand the function V again to second order which leads to

$$g(j) \simeq \langle [\sum_{i\in S} (\nabla\varphi)_i{}^{\perp} - \tfrac{1}{2} J_{XY}]^2 \rangle_{XY}, \tag{21}$$

where $(\nabla\varphi)^{\perp}$ denotes the component of the gradient $\nabla\varphi$ orthogonal to the path S.

Following Kosterlitz[6] one can separate the fluctuations in $\varphi(r)$ into a piece $\bar{\varphi}(r)$ arising from vortex contributions (v) and into a piece $\psi(r)$ connected to the usual spin waves (s). The expression (21) takes then the form

$$g(j) \simeq \langle [\sum_{i\in S} (\nabla\psi)_i{}^{\perp} - \tfrac{1}{2} J_{XY}]^2 \rangle_s + \langle [\sum_{i\in S} (\nabla\bar{\varphi})_i{}^{\perp}]^2 \rangle_v \equiv \Gamma_s(j) + \Gamma_v(j). \tag{22}$$

The vortex term $\Gamma_v(j)$ can be reduced to a more usual form if one passes to the conjugate function $\bar{\varphi}'(r)$ which is connected with $\bar{\varphi}(r)$ through the Cauchy-Riemann relations (compare Ref. 6). Since these relations imply $\nabla\bar{\varphi} \perp \nabla\bar{\varphi}'$, one has

$$\sum_{i\in S} (\nabla\bar{\varphi})_i{}^{\perp} = \sum_{i\in S} (\nabla\bar{\varphi}')_i{}^{\parallel} = \bar{\varphi}'(j) - \bar{\varphi}'(0), \tag{23}$$

and consequently

$$\Gamma_v(j) = \langle [\bar{\varphi}'(j) - \bar{\varphi}'(0)]^2 \rangle_v. \tag{24}$$

Since it is precisely the fields $\bar{\varphi}'(r)$ which lead to the Coulomb-gas formulation of the XY model in the analysis of Ref. 6 one can, using Eq. (2.7) of that reference, directly relate this average to the potential of mean force. The same result was obtained by Chui and Weeks[5] in the case of DG model for the full correlation function $g(j)$. The divergence of $g(j)$ as $\ln|j|$ (above the roughening temperature) following from this identification is recently confirmed by the Monte Carlo simulations of Swendsen.[2]

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[1]G. H. Gilmer and P. Bennema, J. Appl. Phys. 43, 1347 (1972).

[2]R. H. Swendsen, Phys. Rev. Lett. 38, 615(C) (1977).

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

[4]J. D. Weeks, G. H. Gilmer, and H. J. Leamy, Phys. Rev. Lett. 31, 549 (1973).

[5]S. T. Chui and J. D. Weeks, Phys. Rev. B 14, 4978 (1976).

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

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

[8]This relation can be seen as a special case of a more general duality relation obtained recently [R. Savit, Phys. Rev. Lett. 39, 55 (1977)].

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

[10]In general the $\varphi_{j'}$ will be located on the dual lattice of the original one.

[11]This correspondence was also obtained by Villain [J. Villain, J. Phys. (Paris) 36, 581 (1975)] who used a different representation of this interaction that can be obtained from (14) by use of the Poisson summation formula.