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Renormalization Group Theory of the Interfacial Roughening Transition

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The interfacial properties near the roughening transition temperature of the modified discrete Gaussian model in two dimensions are discussed. The interfacial profile is calculated by extending the renormalization group method of Kosterlitz and José et al. The square of the interface width and the inverse of the gradient of the profile at the center are found to be given by $\ln\xi$ and $(\ln\xi)^{1/2}$, respectively, where ξ is the correlation length of fluctuations. These results are different from those of the mean field theory, the low temperature series expansion and those of Müller-Krumbhaar. The cross-over to the mean field results is also discussed. The interfacial profile is obtained and is expressed by the error function. The present results are applicable to the neutral Coulomb gas with a logarithmic interaction and to the classical X-Y model in two dimensions. Therefore the dielectric function near the metal-insulator transition and the spin correlation function above the transition point are also calculated.

§ 1. Introduction

Recently there has been much effort devoted to understanding of the properties of the transition from a localized (smooth) to a delocalized (rough) interface.[5),12)] On the other hand, the interfacial properties based on the Ginzburg-Landau-Wilson Hamiltonian have been investigated by renormalization group methods.[1)] Although many intrinsic properties above three dimensions have been clarified, the results in the absence of some external field cannot be applicable to three dimensions where the unbounded two-dimensional interface is delocalized at all finite temperatures due to the fluctuating capillary waves.[2)~4)] As is well known, one of the methods that resolve this problem is to introduce an external field such as a gravitational field which has the effect of introducing long wavelength cutoff. The other approach is to consider a model which exhibits the transition at a finite temperature in the two-dimensional interface. For a crystal-vapor interface the Solid-On-Solid (SOS) model and the discrete Gaussian (DG) model have been used frequently,[5)] the latter being regarded as a discrete version of the capillary wave theory in fluids.[3)]

In this paper we study the interfacial properties near the roughening transition temperature T_R by means of the renormalization group method of Kosterlitz[6)] and José et al.[7)] The interfacial profile and the associated quantities near T_R, such as the interface width and the gradient of the profile at the center are calculated. Since there is a close relationship among the critical properties of the surface roughening models, the two-dimensional (2-D) Coulomb gas with a logarithmic interaction,[7)~9)] the 2-D classical X-Y model[7),10)] and other systems in low dimensions, the results obtained here are directly applicable to those systems. In particular we discuss the metal-insulator transition of the 2-D Coulomb gas and the spin correlations above the transition point of the 2-D X-Y model.

In § 2 we introduce the model and define the two-point distribution function. In order to calculate the two-point distribution function we introduce an appropriate characteristic function which is manipulated by the Chui-Weeks transformation[8)] and is calculated by a cumulant expansion.

In § 3, following José et al., we construct a set of the renormalization group equations. The interfacial profile is obtained by using the solution of these equations and is compared with the available theoretical results.[5),11),12)] By using the results obtained in § 3, we discuss the transition of the 2-D neutral Coulomb gas in § 4, which is an extension of a simple perturbation approach in terms of fugacity.[13),14)] A universal relationship is derived between the dielectric function at the critical point and the critical exponent η of the 2-D X-Y model. In § 5 we calculate the spin correlation function above the transition point of the 2-D X-Y model. Section 6 is devoted to final remarks and conclusion.

§ 2. Surface roughening model

A simplified model of a 2-D interface is a lattice of columns of height h_i with the following interaction energy:

$$\mathcal{H}\{h\} = \frac{1}{2} J \sum_{i,\delta} (h_i - h_{i+\delta})^2 , \qquad (2\cdot1)$$

where J is a coupling constant. The summation is over all lattice sites i, and the nearest neighbors δ. In a crystal vapor interface the height variables h_i are restricted to integer values $(-\infty < h_i < \infty)$ so that the model (2·1) may be called discrete Gaussian (DG) model. The capillary wave theory in a liquid-vapor interface can also be formally transformed to (2·1)[3)] although there the discreteness of h_i does not play an important role due to the quite small value of $\beta J (\beta = 1/(k_B T))$.

It transpires that the particular renormalization group method we use is better adapted to the modified discrete Gaussian model (MDG) with the following Hamiltonian:

$$\mathcal{H}_M\{h\} = \frac{1}{2} J \sum_{i,\delta} (h_i - h_{i+\delta})^2 - \sum_i \beta^{-1} \ln(1 + 2y_0 \cos 2\pi h_i) , \qquad (2\cdot2)$$

where $|y_0| \leq 1/2$ and h_i is now a continuous real variable. In MDG the lattice periodicity is now taken into account through the periodic potential that appears in the second term of (2·2) rather than by restricting h_i to integer values as in DG. Note that the Chui-Weeks transformation[8)] applies equally well to the MDG and transforms (2·2) to the 2-D Coulomb gas of particles with "charges"

± 1, and $\beta^{-1}\ln y_0$ plays the role of a chemical potential.

In order to see the interfacial properties let us introduce the probability $P(z; \boldsymbol{r}_1-\boldsymbol{r}_2)$ that the height difference of two columns at $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$ on the interface is equal to z as defined by

$$P(z;\boldsymbol{r}_1-\boldsymbol{r}_2)=\langle\delta(z-h_1+h_2)\rangle, \tag{2·3}$$

where

$$\langle A\rangle\equiv\int d\{h\}\,A\,e^{-\beta\mathcal{H}_M}\Big/\int d\{h\}\,e^{-\beta\mathcal{H}_M}. \tag{2·4}$$

The function $P(z;\boldsymbol{r}_{12})$ has an interesting physical meaning. Namely this describes the "conditional" derivative profile of the interface in the column of site 2 when the interface in the column of site 1 is fixed at $z=0$. Note that z stands for the coordinate perpendicular to the interface.

It is convenient to express $P(z;\boldsymbol{r}_{12})$ using a characteristic function $E(k;\boldsymbol{r}_{12})$ as

$$P(z_{12};\boldsymbol{r}_{12})=\frac{1}{2\pi}\int_{-\infty}^{\infty}dk\,e^{ik(z_1-z_2)}E(k;\boldsymbol{r}_{12}) \tag{2·5}$$

with

$$E(k;\boldsymbol{r}_{12})=\langle e^{-ik(h_1-h_2)}\rangle, \tag{2·6}$$

where $\boldsymbol{r}_{12}$ denotes a vector parallel to the interface directed from site 1 to site 2. From the definition (2·6) the characteristic function satisfies the following relations:

$$E(k;\boldsymbol{r}_{12})=E(-k;\boldsymbol{r}_{12}). \tag{2·7}$$

The characteristic function $E(k;\boldsymbol{r}_{12})$ is reexpressed by using the transformation of Chui and Weeks[8] with the following result:

$$E(k;\boldsymbol{r}_{12})=\exp\left[-\frac{k^2}{4\pi\beta J}G_0(\boldsymbol{r}_1-\boldsymbol{r}_2)\right]$$

$$\times\left\langle\exp\left[\frac{k}{4\pi\beta J}\sum_{\boldsymbol{r}}2\pi m(\boldsymbol{r})\,\{G_0(\boldsymbol{r}-\boldsymbol{r}_1)-G_0(\boldsymbol{r}-\boldsymbol{r}_2)\}\right]\right\rangle_e, \tag{2·8}$$

where $\langle\cdots\rangle_e$ is the canonical average,

$$\langle A\rangle_e=\sum_{\{m\}}A\,y_0^{\,N}\,e^{-\beta^{-1}\mathcal{H}_e}\Big/\sum_{\{m\}}y_0^{\,N}\,e^{-\beta^{-1}\mathcal{H}_e} \tag{2·9}$$

with the Hamiltonian

$$\mathcal{H}_e=-\frac{\pi}{2J}\sum_{\boldsymbol{r},\boldsymbol{r}'}m(\boldsymbol{r})\,m(\boldsymbol{r}')\,G_0(\boldsymbol{r}-\boldsymbol{r}'). \tag{2·10}$$

Here $m(\boldsymbol{r})=0,\ \pm 1$, and $N\equiv\sum_{\boldsymbol{r}} m(\boldsymbol{r})^2$ is the total number of particles. The potential $G_0(\boldsymbol{r})$ is given for a lattice with the lattice constant a_0 by

$$G_0(\boldsymbol{r})=2\pi a_0^2\int_{\boldsymbol{q}}\frac{1-e^{i\boldsymbol{q}\cdot\boldsymbol{r}}}{4-2\cos(q_x a_0)-2\cos(q_y a_0)} \tag{2·11}$$

and

$$\int_{\boldsymbol{q}}\equiv\int\frac{d^2\boldsymbol{q}}{(2\pi)^2}. \tag{2·12}$$

The system is now equivalent to the 2-D neutral Coulomb gas with integral charges $m(\boldsymbol{r})$ on the lattice whose Hamiltonian is (2·10). Note, however, that the temperature β in the 2-D Coulomb gas is inversely related to the temperature β^{-1} of the original DG model.[7),8)] The characteristic function (2·8) is obtained by introducing a pair of "test charges" $k/2\pi$ and $-k/2\pi$ at $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$ respectively, in the Coulomb gas.

Following José et al.,[7)] we calculate Eq. (2·8) by using a cumulant expansion. The characteristic function is then obtained up to first order in this expansion as

$$E(k;\boldsymbol{r}_{12})=\exp\left[-\frac{k^2}{4\pi\beta J}G(\boldsymbol{r}_1-\boldsymbol{r}_2)\right], \tag{2·13}$$

where $G(\boldsymbol{r})$ is an effective interaction potential and is expressed as

$$G(\boldsymbol{r})=G_0(\boldsymbol{r})-\frac{\pi}{2\beta J}\sum_{\boldsymbol{R},\boldsymbol{r}'}\langle m(0)\,m(\boldsymbol{r}')\rangle_e\left(G_0\left(\boldsymbol{R}+\boldsymbol{r}+\frac{\boldsymbol{r}'}{2}\right)-G_0\left(\boldsymbol{R}+\frac{\boldsymbol{r}'}{2}\right)\right)$$
$$\times\left(G_0\left(\boldsymbol{R}+\boldsymbol{r}-\frac{\boldsymbol{r}'}{2}\right)-G_0\left(\boldsymbol{R}-\frac{\boldsymbol{r}'}{2}\right)\right). \tag{2·14}$$

The second term contributes to the screening of the potential by fluctuating charges. Defining Fourier transform by $G(\boldsymbol{r})=a_0^2\int_{\boldsymbol{q}}(1-e^{i\boldsymbol{q}\boldsymbol{r}})G(\boldsymbol{q})$ as in (2·11) and regarding the second term of (2·14) as a self-energy, we obtain from (2·14)

$$G(\boldsymbol{q})=\frac{G_0(\boldsymbol{q})}{1-(\pi/\beta J)\sum_{\boldsymbol{r}}\langle m(0)\,m(\boldsymbol{r})\rangle_e(1-e^{i\boldsymbol{q}\boldsymbol{r}})G_0(\boldsymbol{q})}, \tag{2·15}$$

where

$$G_0(\boldsymbol{q})=2\pi[4-2\cos(q_x a_0)-2\cos(q_y a_0)]^{-1}.$$

The denominator of (2·15) is directly related to the dielectric function of the 2-D Coulomb gas. We shall discuss this point separately in § 4.

Before applying the renormalization group procedure to (2·15), we derive the expressions of some quantities associated with the interfacial profile. The derivative profile is given from (2·5) and (2·13) by

$$P(z;\boldsymbol{r}) = [\pi/KG(\boldsymbol{r})]^{1/2} \exp\left[-\frac{\pi^2 z^2}{KG(\boldsymbol{r})}\right] \tag{2·16}$$

with

$$K=\pi/(\beta J).^{*)}$$

The gradient of the profile at the center M is, then, obtained by

$$M \equiv \lim_{r\to\infty} P(0;\boldsymbol{r}) = \lim_{r\to\infty}\left\{\frac{K}{\pi}G(\boldsymbol{r})\right\}^{-1/2}. \tag{2·17}$$

Here we have assumed that $G(\boldsymbol{r})$ is sufficiently large for $r\to\infty$. The interface width L is obtained through the second moment $g(\boldsymbol{r})$ of the derivative profile $P(z;\boldsymbol{r})$:[8]

$$L^2 = \lim_{r\to\infty} g(\boldsymbol{r}) \tag{2·18}$$

with

$$g(\boldsymbol{r}) \equiv \int_{-\infty}^{\infty} dz\, z^2 P(z;\boldsymbol{r}) = \langle (h(0)-h(\boldsymbol{r}))^2\rangle = \frac{K}{2\pi^2}G(\boldsymbol{r}). \tag{2·19}$$

In the subsequent section we analyze the effective potential (2·15) employing the renormalization group method and obtain the temperature and the $\boldsymbol{r}$ dependence of $P(z;\boldsymbol{r})$, M and L.

§ 3. Renormalization group equations and interfacial properties

3.1. *Renormalization group equations*

José et al. have constructed a set of recursion relations in the limit $q\to 0$ of the denominator of Eq. (2·15). It is appropriate only above the roughening transition temperature T_R (below the transition point of the 2-D X-Y model and the 2-D Coulomb gas). The system they considered reduces to ours if multiply charged particles allowed in their system are ignored which they seem to do at low temperatures of the 2-D Coulomb gas.[7] Now, below T_R, on the other hand, one cannot discard the q-dependence, which is crucial in determining the interfacial properties.

Let us rewrite (2·15) as

$$KG(\boldsymbol{q}) = G_0(\boldsymbol{q})/Q(\boldsymbol{q}), \tag{3·1}$$

where

$$Q(\boldsymbol{q}) = K^{-1} - \sum_{\boldsymbol{r}} \langle m(0)\, m(\boldsymbol{r})\rangle_e (1-e^{i\boldsymbol{qr}})\, G_0(\boldsymbol{q}) \tag{3·2}$$

and K has been defined in the previous section. The average $\langle m(0)\, m(\boldsymbol{r})\rangle_e$ is

*) Our K is equal to $2\pi K$ of José et al.[7]

obtained by José et al. to be

$$\langle m(0)\,m(\boldsymbol{r})\rangle_e = -2y_0^2 e^{-KG_0(\boldsymbol{r})} = -2y^2(r/a_0)^{-K} \tag{3·3}$$

with

$$y = y_0 e^{-(\pi/4)K}. \tag{3·4}$$

Although this result was obtained at low temperatures of the 2-D X-Y model, the same result holds for the 2-D Coulomb gas in wider temperature regions except in the metallic region and in the immediate vicinity of the transition as long as the fugacity y is sufficiently small.[14]

It is appropriate here to discuss the scaling law for $\langle m(0)\,m(\boldsymbol{r})\rangle_e$ based on the dimensional analysis. Define

$$S(\boldsymbol{r}, a_0, K, y) = \langle m(0)\,m(\boldsymbol{r})\rangle_e, \tag{3·5}$$

where the dependence of S on the cutoff a_0 and K and y is explicitly indicated. Let us now change the unit of length so that $a_0 \to a_0 e^l$. This will give rise to the following changes:

$$\boldsymbol{r} \to e^l \boldsymbol{r}, \quad y \to y(l), \quad K \to K(l), \tag{3·6}$$

where $y(l)$ and $K(l)$ will be obtained below by solving a renormalization group equation. Since S is dimensionless ($m(\boldsymbol{r})$ is dimensionless), S should remain the same under this length change. Therefore we have

$$S(\boldsymbol{r}, a_0, K, y) = S(e^l \boldsymbol{r}, e^l a_0, K(l), y(l)). \tag{3·7}$$

Using the perturbation theory result (3·3) on the right-hand side of (3·7), we thus obtain

$$\langle m(0)\,m(\boldsymbol{r})\rangle_e = -2y(l)^2 (r/a_0)^{-K(l)}. \tag{3·8}$$

The use of this form is justified for large l since repeated applications of the RG transformation bring the system well outside the transition region and $y(l)$ turns out to be not greater than $1/4\pi$ (see the sentence after (3·25)).

Now, we construct a set of the renormalization group equations. First let us consider the renormalization of K^{-1} in (3·2). For this purpose we define

$$K(\boldsymbol{q}, l)^{-1} = K^{-1} - \frac{(2\pi)^2}{q^2 a_0^4} \int_{a_0}^{a_0 e^l} dr\, r \langle m(0)\,m(r)\rangle_e [1 - J_0(qr)] \tag{3·9}$$

and

$$K(l)^{-1} \equiv K(0, l)^{-1}, \tag{3·10}$$

where $J_0(x)$ is the Bessel function of the first kind. The function $Q(q)$ is then obtained by

$$Q(q) = K(q, \infty)^{-1}, \tag{3·11}$$

where we have used a continuum approximation $G_0(q) = 2\pi/(qa_0)^2$. $K(l)^{-1}$ given by (3·10) is evidently the same as that introduced in (3·6) by its definition. Differentiating (3·9) with respect to l, we obtain

$$\frac{\partial}{\partial l}K(q, l)^{-1} = \frac{8\pi^2 y(l)^2}{(qa_0e^l)^2}[1 - J_0(qa_0e^l)] \tag{3·12}$$

with

$$y(l)^2 \equiv -\frac{1}{2}e^{4l}\langle m(0)\, m(a_0e^l)\rangle_e . \tag{3·13}$$

Similarly we have from (3·10)

$$\frac{\partial}{\partial l}K(l)^{-1} = 2\pi^2 y(l)^2 . \tag{3·14}$$

In order to obtain the equation for $y(l)$ we construct the ratio

$$\frac{y(l+\delta l)^2}{y(l)^2} = e^{4\delta l}\frac{\langle m(0)\, m(a_0e^{l+\delta l})\rangle_e}{\langle m(0)\, m(a_0e^l)\rangle_e} . \tag{3·15}$$

By substituting the scaling law result (3·8) into the right-hand side of (3·15), we have

$$y(l+\delta l)^2/y(l)^2 = \exp\{\delta l[4 - K(l)]\}$$

which can be converted to the following by letting $\delta l \to 0$:

$$\frac{\partial}{\partial l}y(l)^2 = (4 - K(l))\, y(l)^2 . \tag{3·16}$$

The renormalization group equations (3·14) and (3·16) which are rewritten as

$$\frac{\partial x^2}{\partial l} \simeq -xz^2 , \quad \frac{\partial z^2}{\partial l} = -xz^2 \tag{3·17}$$

with

$$x = K - 4 , \tag{3·18}$$

$$z = 8\pi y , \tag{3·19}$$

have been analyzed by Kosterlitz[6] and Wegner.[15] The RG trajectory is displayed in Fig. 1. There is a conserved quantity:

$$x^2 - z^2 = c^2 t , \tag{3·20}$$

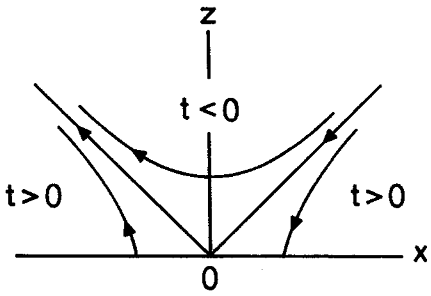

Fig. 1. The RG trajectory determined by (3·17).

where c is some positive constant and t stands for the reduced temperature $(T-T_R)/T_R$.*)

Above $T_R(t>0)$**) the variable y is shown to be irrelevant. Therefore the effective potential $G(\boldsymbol{r})$ behaves in a manner similar to $G_0(\boldsymbol{r})$, i.e., $G(\boldsymbol{r})\propto G_0(\boldsymbol{r})\sim\ln(r/a_0)$ for large r. The interface width L defined by (2·18) is thus always infinite.[8] The solutions of (3·17) below $T_R(t<0)$ are written as[6),15)]

$$x(l)=c\sqrt{|t|}\tan\psi(l), \tag{3·21}$$

$$z(l)=c\sqrt{|t|}\sec\psi(l) \tag{3·22}$$

with

$$\psi(l)=\psi(0)-c\sqrt{|t|}\,l/2, \tag{3·23}$$

(3·21) is written inversely as

$$l=\frac{2}{c\sqrt{|t|}}\left\{\tan^{-1}\left(\frac{x(0)}{c\sqrt{|t|}}\right)-\tan^{-1}\left(\frac{x(l)}{c\sqrt{|t|}}\right)\right\}, \tag{3·24}$$

where we choose the branch of $\tan^{-1}$ to be $-\pi/2<\tan^{-1}<\pi/2$. If we integrate Eqs. (3·17) up to $l=l^*$ such that $-2<x(l^*)<0$,***) we may approximate (3·24) for sufficiently small $|t|$ as

$$l=\begin{cases}0 & \text{for } x(l)>0,\\ l^* & \text{for } x(l)<0,\end{cases} \tag{3·25}$$

since $x(0)>0$ for $T<T_R$. Note that $|x(l^*)|<2$ implies $y<1/4\pi$ for very small t.

By using (3·17), (3·19) and (3·24) we can solve Eq. (3·12). The function $Q(q)$ for $t<0$ is then obtained by using the relation (3·11) as

$$Q(q)=\frac{x}{16}+\frac{|x^*|}{4(q\xi)^2}(1-J_0(q\xi))+[K^{-1}(q,l=\infty)-K^{-1}(q,l=l^*)+K^{-1}] \tag{3·26}$$

with $x=x(0)$, $x^*=x(l^*)$. We choose l^* such that the correlation length ξ of

*) See also the discussion at the end.

**) Here and after we exclude the region $x(0)+y(0)\leq 0$.

***) Note from (3·18) that this region corresponds to $2<K<4$. We have an exact solution for $K<2$. For example in the terminology of the 2-D Coulomb gas the dielectric function for $K<2$ obeys exactly the Debye-Hückel form in the low density limit (see § 4).

fluctuations which transforms as $\xi(l)=e^{-l}\xi(0)$ is given by $\xi=\xi(0)=a_0 e^{l^*}$. Then we obtain[6]

$$\xi=a_0\, e^{c_1/\sqrt{|t|}}\,, \tag{3·27}$$

where $c_1\equiv 2\pi/c$. The term in [ ] of (3·26) to be denoted as $Q^*(q\xi)$ is to be calculated outside the critical region and is written as

$$Q^*(q\xi)=K^{-1}+\Delta Q(q\xi)\,, \tag{3·28}$$

where we expect that $\Delta Q(x)$ vanishes rapidly for $x\gg 1$. This point will be discussed again in § 4. Substituting (3·28) into (3·26), we finally obtain ignoring a term of $O(x^2/64)$,

$$Q(q)=\frac{1}{4}+\frac{|x^*|}{4(q\xi)^2}(1-J_0(q\xi))+\Delta Q(q\xi)\equiv\widehat{Q}(q\xi)\,. \tag{3·29}$$

3.2. *Interfacial properties*

We are now in a position to discuss the interfacial properties. The effective potential in real space is found from (3·1) and (3·29) and also noting that $KG(\boldsymbol{r})=a_0^2\int_{\boldsymbol{q}}KG(\boldsymbol{q})\,(1-e^{i\boldsymbol{qr}})$ with the following result:

$$KG(\boldsymbol{r})=\int_0^{\xi/a_0}dx\frac{1}{x}\{1-J_0(xr/\xi)\}\frac{1}{\widehat{Q}(x)}\,. \tag{3·30}$$

In the limit $r/\xi\to\infty$ and for $\xi/a_0\gg 1$, $KG(\boldsymbol{r})$ behaves as

$$KG(\boldsymbol{r})\simeq 4\ln(\xi/a_0) \tag{3·31}$$

since $\widehat{Q}(x)$ tends to 1/4 as $x\to\infty$. In contrast to above T_R where $G(\boldsymbol{r})$ grows as $\ln(r/a_0)$,[8] the effective potential below T_R is thus bounded from above. The interface width (2·18) is then obtained by

$$L^2=\frac{2}{\pi^2}\ln(\xi/a_0)=\frac{4}{\pi c}|t|^{-\theta_2} \tag{3·32}$$

with $\theta_2=1/2$, where we have used (3·27). Needless to say, ξ is not to be confused with the bulk correlation length in three dimensions but the interface correlation length associated with the fluctuations of the Hamiltonian (2·2). The higher moments are also calculated as

$$\langle z^{2k}\rangle\equiv\int_{-\infty}^{\infty}dz\, z^{2k}P(z;\infty)\propto|t|^{-k/2}\,. \tag{3·33}$$

The gradient of the profile at the center M is similarly obtained from (2·17) by

$$M^{-1}=\left\{\frac{4}{\pi}\ln(\xi/a_0)\right\}^{1/2}\propto|t|^{-\theta_M} \tag{3·34}$$

with $\theta_M=1/4$. Finally the profile $\rho(z)$ is given choosing $\rho(+\infty)=0$ by

$$\rho(z)=\int_z^\infty dz' P(z';\infty)$$
$$=\frac{1}{2}\{1-\mathrm{erf}(z/(\sqrt{2}L))\}, \tag{3·35}$$

where we have used (2·16). The error function is defined by

$$\mathrm{erf}(x)=\frac{2}{\sqrt{\pi}}\int_0^x e^{-t^2}dt. \tag{3·36}$$

The exponents obtained here are different from those of the mean field theory[11] and the low temperature expansion results[12] and those of Müller-Krumbhaar[5] (see Table I). Although we cannot claim that our critical exponents are exact, each of the treatments referred to above also is not free from its own shortcomings. First there is no reason that the present results should agree with the mean field results.[11] The low temperature series expansion results have been criticized because the exponents obtained do not satisfy the Lapunov inequality.[16] It is interesting to note that our exponents satisfy the Lapunov inequality as the equality just as the mean field values. Müller-Krumbhaar used an alternative renormalization group method of Coleman.[17] In evaluating the exponents, however, a variational approximation was employed,[5] the validity of which is also unclear.

From the view point of a scaling law the effective potential (3·31) is nicely matched to $KG(\boldsymbol{r})\simeq 4\ln(r/a_0)$ for $T>T_R$, where the present renormalization group method is well understood. For $T<T_R$, the scaling field y turns out to be relevant. Thus the use of (3·8) can be problematical there. However, the smallness of $y(l)$ $(<1/4\pi)$ for $l\simeq l^*$ justifies our use of (3·8). On the other hand, there is an analogous situation in the antiferromagnetic case of the Kondo problem discussed in detail by Anderson et al.,[15] the results of which are well established. Kosterlitz[6] briefly discussed the Y-X model above the transition using the same approximation.

Before concluding this section we wish to make two important observations. First, we note that y is the parameter that measures the breakdown of the translation invariance in the direction perpendicular to the interface. The fact that y

Table I. The exponents obtained by the various methods.

	θ_M	θ_2	θ_4
Mean field theory[11]	1/2	1	2
Low temperature series expansion			
{ isotropic Ising ferromagnet[12]	0.78	1.00	1.43
{ SOS model[12],[16]	0.972	0.968	—
by Müller-Krumbhaar[5]	1/2	1	2
This work	1/4	1/2	1

is relevant below T_R and is irrelevant above T_R implies that the translation invariance which is broken below T_R gets restored above T_R.*) The second point is concerned with the relationship of our results with those of the mean field theory. First we note that the critical line (K_R, y_{0R}) is given by using (3·4), (3·18), (3·19), (3·20) with $t=0$ and $l=0$ as

$$K_R - 8\pi y_R = 4 \tag{3·37}$$

with

$$y_R = y_{0R} e^{-(\pi/4)K_R}. \tag{3·38}$$

The critical line ends at the fixed point $K^*=4$ and $y_R^* = y_{0R}^* = 0$. Now, (3·17) says that $x^2 - y^2$ is independent of l. Thus $x(l)^2 - z(l)^2 = x(0)^2 - z(0)^2$. In (3·20) we expanded the right-hand side in powers of t and retained only the first term. We here examine this point more carefully by writing $x(0)^2 - z(0)^2$ out using (3·37) as

$$\begin{aligned} x(0)^2 - z(0)^2 &= [K(0)-4]^2 - [8\pi y(0)]^2 - (K_R - 4)^2 + (8\pi y_R)^2 \\ &= 2(K_R - 4)[K(0) - K_R] - 2(8\pi)^2 y_R [y(0) - y_R] \\ &\quad + [K(0) - K_R]^2 - (8\pi)^2 [y(0) - y_R]^2 . \end{aligned} \tag{3·39}$$

If the initial point $(K(0), y(0))$ is near a point (K_R, y_R) on the critical line which is not near the fixed point, the first line of (3·39) dominates and we have (3·20). On the other hand, as (K_R, y_R) approaches the fixed point $(4, 0)$, c^2 in (3·20) tends to zero and the second line of (3·39) cannot be ignored. In this case (3·39) becomes

$$x(0)^2 - z(0)^2 \cong c^2 t - d^2 \cdot t^2 \tag{3·40}$$

with

$$c^2 = 2(K_R - 4) K_R' - 2(8\pi)^2 y_R y_R' , \tag{3·41}$$

$$d^2 = (K_R')^2 - (8\pi)^2 (y_R')^2 , \tag{3·42}$$

where $K_R' = [dK/dt]_R$ etc. Here we should note that (3·40) must be negative for $t<0$. Thus we expect the crossover: The mean field critical exponents for $-t > c^2/d^2$ and the present critical exponents for $-t < c^2/d^2$. There is, however, one difficulty. Namely, (3·40) predicts that there are two critical temperatures associated with the critical line $x(0) = z(0)$: $t=0$ and $t = c^2/d^2 \ll 1$. At the moment we have not understood the implication of this peculiar fact.

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*) This should not be confused with the spontaneous break-down of symmetry since the starting Hamiltonian is *not* translationally invariant.

§ 4. Dielectric function of 2-D Coulomb gas

Table II. Correspondence among the notations of the MDG model, the 2-D Coulomb gas and the 2-D X-Y model.

	MDG model	Coulomb gas[14]	X-Y model[7]
K	$\pi/(\beta J)$	βe^2	$2\pi\beta J$
y	$y_0 e^{-\pi^2/(4\beta J)}$	fugacity	$y_0 e^{-\pi^2\beta J/2}$

The results derived in the previous section are also applicable to the 2-D Coulomb gas system with the Hamiltonian (2·9). Especially the function $KQ(\boldsymbol{q})$ with $Q(\boldsymbol{q})$ given by (3·2) is interpreted as the dielectric function $\varepsilon(\boldsymbol{q}, T)$ of this system provided that β is replaced by β^{-1}. In fact it is readily shown that (3·2) is calculated in the low density regime from the formula

$$\varepsilon(\boldsymbol{q}, T) = 1 + \frac{2\pi\beta}{q^2} F(\boldsymbol{q}, T), \tag{4·1}$$ *)

where $F(\boldsymbol{q}, T)$ is the charge density correlation function.[14] The correspondence of the notations among the MDG model, the 2-D Coulomb gas and the 2-D X-Y model are summarized in Table II.

The 2-D Coulomb gas system behaves like a neutral gas of bound pairs of charges of opposite sign at low temperatures and exhibits the metallic behavior of a plasma at high temperatures.[18),19)] Between these insulating and metallic states there is an intermediate region,[14] the lowest temperature T_c of which corresponds to the roughening transition temperature T_R of the MDG model.

Below T_c we may neglect the $\boldsymbol{q}$-dependence of $\varepsilon(\boldsymbol{q}, T)$. Applying the renormalization group method, we easily obtain near T_c

$$(\beta e^2)^{-1}\varepsilon(T) = 1/4 - c_2\sqrt{|\tau|}, \tag{4·2}$$

where c_2 is some positive constant and $\tau = (T-T_c)/T_c$. The $\sqrt{|\tau|}$ dependence has been obtained by Kosterlitz.[6] It is interesting to note that the universal value 1/4 of $(\beta e^2)^{-1}\varepsilon(T)$, when T_c is approached from below, is directly related to the critical exponent η of the 2-D X-Y model[6),7)] (see also § 5). This is analogous to a universal jump of the superfluid density in helium film discussed by Nelson and Kosterlitz.[20]

Above T_c the dielectric function is obtained by re-interpretation of (3·29) as

$$(\beta e^2)^{-1}\varepsilon(\boldsymbol{q}, T) = \frac{1}{4} + \frac{|x^*|}{4(q\xi)^2}(1 - J_0(q\xi)) + \frac{c_3}{(q\xi)^2}, \tag{4·3}$$

where c_3 is some positive constant. Here we have chosen the Debye-Hückel form for $Q^*(q\xi)$ given by (3·28), which is exact for the sufficiently high temperature regime.[18] Of course (4·3) does not agree with the simple perturbation result.[14]

*) Here the Hamiltonian of the 2-D Coulomb gas is defined by (2·10) with the correspondence $\pi/(\beta J) \Leftrightarrow \beta e^2$, $e = \pm 1$ being a charge. The potential $G_0(\boldsymbol{r})$ then obeys the equation $\nabla^2 G_0(\boldsymbol{r}) = 2\pi\delta(\boldsymbol{r})$. The factor 2π in (4·1) rather than the usual 4π is chosen to be consistent with this definition.

§ 5. Spin correlations of 2-D X-Y model

Using the results obtained in § 3, we study the spin correlation function above T_c of the 2-D classical X-Y model with the Hamiltonian:

$$\mathcal{H}_{XY}=J\sum_{\langle \boldsymbol{r},\boldsymbol{r}'\rangle}\{1-\cos[\theta(\boldsymbol{r})-\theta(\boldsymbol{r}')]\}, \tag{5·1}$$

where the summation $\langle \boldsymbol{r},\boldsymbol{r}'\rangle$ is over the nearest neighbor sites on a two-dimensional lattice. $\theta(\boldsymbol{r})$ is the angle that the spin $\boldsymbol{S}(\boldsymbol{r})$ ($|\boldsymbol{S}|=1$) makes with some arbitrary axis. The correlation function $g_p(\boldsymbol{r})$ is then defined by

$$g_p(\boldsymbol{r}-\boldsymbol{r}')=\langle e^{i[\theta(\boldsymbol{r})-\theta(\boldsymbol{r}')]}\rangle. \tag{5·2}$$

José et al.[7] reduce the problem to a Coulomb gas system and approximately evaluate $g_p(\boldsymbol{r})$ which is in the present notations

$$g_p(\boldsymbol{r})=\exp[-G_0(\boldsymbol{r})/K_{\rm eff}], \tag{5·3}$$

where

$$K_{\rm eff}^{-1}=K^{-1}-\frac{\pi}{2}\sum_{\boldsymbol{r}_0}r_0^2\langle m(0)\,m(a_0\boldsymbol{r}_0)\rangle_e\,. \tag{5·4}$$

Equation (5·4) has been obtained by a gradient expansion approximation. It should be noted that $Q(q)$ given by (3·2) agrees with (5·4) in the limit $q\to 0$. Therefore we can generalize (5·3) using $Q(q)$ as

$$g_p(\boldsymbol{r})=\exp\left[-a_0^2\int_{\boldsymbol{q}}G_0(\boldsymbol{q})\,Q(\boldsymbol{q})\,(1-e^{i\boldsymbol{q}\boldsymbol{r}})\right]. \tag{5·5}$$

By making use of (3·29) for $Q(q)$, Eq. (5·5) is easily calculated to be

$$g_p(r)\simeq g_p{}'(r/\xi)\left(\frac{r}{a_0}\right)^{-1/4}\exp\left[-\frac{|x^*|}{4}R(r/\xi)\right], \tag{5·6}$$

where

$$R(x)=\int_0^\infty dz\,z^{-3}(1-J_0(z))\,(1-J_0(xz)). \tag{5·7}$$

This integral is performed analytically[21] as

$$R(x)=\begin{cases}\dfrac{1}{4}(\ln x+1) & \text{for}\quad x>1\,,\\[2ex] \dfrac{x^2}{4}(1-\ln x) & \text{for}\quad x<1\,.\end{cases} \tag{5·8}$$

The function $g_p{}'(r/\xi)$ which comes from the term $\Delta Q(q\xi)$ in (3·23) is to be calculated in the high temperature regime, e.g., by a high temperature series expansion. The correlation $g_p(r)$ for $r>\xi$ precisely agrees with that obtained by Kosterlitz.[6] However, the form of $R(x)$ for $x<1$ obtained here is a new result. At first sight the result (5·6) as well as the corresponding result of Kosterlitz appears to depend on x^* which becomes increasingly arbitrary as $t\to 0$. However, in fact ΔQ and hence g_p' should also depend on x^* in such a way that this arbitrariness disappears.

§ 6. Concluding remarks

In the preceding sections we have investigated the critical properties of the MDG model, the 2-D Coulomb gas and the 2-D classical X-Y model within the renormalization group method of Kosterlitz. Using the function $Q(q)$ given by (3·2), the interface width, the dielectric function and the spin correlation function in the respective systems are studied in a unified way. The spin correlation function for $r>\xi$ of the X-Y model is in agreement with that of Kosterlitz. The dielectric function above T_c obtained in § 4 is a new result, and below T_c it is consistent with that of Kosterlitz. The interfacial properties obtained in § 3, however, does not agree with those of the previous results obtained by the different methods.[5),11),12)] Although the above mentioned agreements in the Coulomb gas and the X-Y model are quite encouraging, one of the tests of the results (3·32)$\sim$(3·34) will be provided by precise computer simulation of interface models.

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