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1987 J. Phys. A: Math. Gen. 20 5619

(http://iopscience.iop.org/0305-4470/20/16/035)

J. Phys. A: Math. Gen. **20** (1987) 5619-5625. Printed in the UK

Scaling in the solid-on-solid interface

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Received 18 February 1987

Abstract. The explicit forms of the density-density correlation function $H(\Delta x, z_1, z_2)$ for the transverse separation $\Delta x \sim W^2$, where W is the interface thickness, are obtained in the two-dimensional solid-on-solid model in two different asymptotic cases of a finite system in a vanishing external field. The results support the Weeks scaling hypothesis. The form of $H_s(\Delta x/\xi_{\perp}, z_1/W, z_2/W)$ depends on the geometry of the system. The relation between W and transverse correlation length $\xi_{\perp}$ has the same form in different external conditions localising the interface in solid-on-solid and capillary-wave models.

1. Introduction

The structure of the fluctuating interface may be studied from different points of view. In one approach, the intrinsic local structure of the interface is investigated. It was found that the bare density profile [1-5] and the conditional correlation functions [6-8] vary on the microscopic scale independent of the method of localising the interface and exist in the limit of unbounded interface fluctuations [1-8].

In this paper we focus our attention on another aspect of the problem of the interface structure. We are interested in the effect of the external conditions stabilising the interface on the distribution of the matter described by the density profile $\rho(\boldsymbol{r}) = \rho(z)$ and the density-density correlation function $H(\boldsymbol{r}_1, \boldsymbol{r}_2) = H(\Delta x, z_1, z_2)$. The interface may be localised in the presence of the bulk external field g or in the finite system, say in a box $L^{d-1} \times M$, where M is the size of the system in the longitudinal direction. The asymptotic cases of $L = \infty$, $M < \infty$ or $L < \infty$, $M = \infty$ with the interface pinned to the walls, in which the interface is still localised, differ from each other because of the anisotropy of the interface region. ρ and H depend on the interparticle potential and on the way the interface is localised. In the strongly fluctuating interface some properties of ρ and H are expected to be universal [9, 10].

The exact results obtained for ρ in lattice models [6, 11-13] and capillary-wave theory [14, 15] suggest that ρ is of the scaling form

$$\rho(z) = \rho_s(z^*) \qquad z^* = z/W \tag{1}$$

where the interface thickness W depends on the way the interface is localised and, in the different asymptotic cases, is given by the expressions (for $d = 2$)

$$W = \begin{cases} (2g\beta\Gamma)^{-1/4} & g \neq 0,\ L = M = \infty;\ \text{SOS [12, 13], capillary waves [15]} \\ [L/(2\beta\Gamma)]^{1/2} & g = 0,\ M = \infty,\ L < \infty;\ \text{lattice gas [1], SOS [6], capillary waves [15]} \\ 2(M+1)/\pi & g = 0,\ M < \infty,\ L = \infty;\ \text{SOS [6]} \end{cases} \tag{2}$$

where the effective surface tension Γ is defined in [16] and $\beta=(kT)^{-1}$ with T the temperature and k the Boltzmann constant.

The explicit forms of $\rho_s(z^*)$ have been found to be as follows:

$$\rho_s(z^*)=\begin{cases}\frac{1}{2}(\rho_l+\rho_g)-(\rho_l\rho_g)\,\mathrm{erf}(z^*) & g\neq 0 \text{ or } L<\infty\ [6, 11\text{–}15]\\ \frac{1}{2}-[z^*+\frac{1}{2}\sin(2z^*)]/\pi & M<\infty\ [6].\end{cases} \tag{3}$$

In the above the function erf is given by

$$\mathrm{erf}(x)=\frac{1}{\sqrt{\pi}}\int_0^x \mathrm{d}t\,\mathrm{e}^{-t^2}.$$

For $d=2$ the explicit form of H has been found in the case of $g\neq 0$ in the capillary wave model to be

$$H(\Delta x, z_1, z_2)=\begin{cases} f(\Delta x)p_s(z_1^*)p_s(z_2^*) & \Delta x\to\infty \qquad (4a)\\ (\rho(z_{\max})-\rho_v)(\rho_l-\rho(z_{\min})) & \Delta x\to 0 \qquad (4b)\end{cases}$$

where $f(x)\to 0$ for $x\to\infty$ and $z_{\max}=z_i$, $z_{\min}=z_j$ if $z_i>z_j$ with $i,j=1,2$, ρ_v and ρ_l are vapour and liquid densities respectively, and

$$p_s(z^*)=-\mathrm{d}\rho_s(z^*)/\mathrm{d}z^*. \tag{5}$$

In the case of $g=0$, H has been found for $d=2$ in the sos model [6] in both asymptotic cases [6]. The results, limited to the case of $\Delta x=\mathrm{o}(W^2)$ are of the form (4*b*).

Recently, Weeks [9] has suggested that in the interface region H is, for $d<3$ and for $\Delta x\gg\xi_1(g)$, of the scaling form

$$H(\Delta x, z_1, z_2)=H_s(\Delta x^*, z_1^*, z_2^*) \qquad \Delta x^*=\Delta x/\xi_\perp(g) \qquad z^*=z/W. \tag{6}$$

Here $\xi_\perp$ is the length unit in the direction perpendicular to the field g inducing the phase separation.

This hypothesis is based on the postulate that in the interface region the only independent relevant length is the capillary wavelength

$$\xi_\perp^2(g)=\Gamma/[(\rho_l-\rho_v)mg] \tag{7}$$

related to W according to the following expression:

$$W^2\sim\xi_\perp^{3-d}(g). \tag{8}$$

The above scaling hypothesis has been verified in the capillary-wave model [15]. In the case of $g=0$, $\xi_\perp(g)$ ceases to be a characteristic length. In the finite system the interface is however localised and one may expect that H has the scaling form (6) with W given by (2) and with $\xi_\perp(g)$ replaced by the transverse correlation length $\xi_\perp$ depending on L and/or M. The results of [6] support the postulate that W is the length unit in the longitudinal direction but are limited to $\Delta x=\mathrm{o}(W^2)$, whereas in view of (7) it is plausible that $\xi_\perp=\mathrm{O}(W^2)$ $(d=2)$.

In this paper we extend the results of [6] to the case of $\Delta x=\mathrm{O}(W^2)$. The explicit forms of H show that, for $d=2$, in both asymptotic cases the scaling hypothesis is verified with $\xi_\perp(g)$ replaced by $\xi_\perp(L)$ or $\xi_\perp(M)$ which arise in a natural way from exact calculations. $\xi_\perp(L)$ or $\xi_\perp(M)$ satisfy the same relation as $\xi_\perp(g)$ in the capillary-wave model [15]:

$$\xi_\perp^2 W^{-1}=2\beta\Gamma \qquad \text{for } d=2. \tag{9}$$

This relation depends only on the surface tension and is of the same form in different external conditions and in different models (for example, sos and capillary waves), and thus seems to be a universal property of the interface.

2. Explicit form of $H(\Delta x, z_1, z_2)$ for $\Delta x = O(W^2)$ in the SOS (solid-on-solid) model

The configuration space of the SOS model consists of the sequences (h_i) of integer heights. The probability of configuration (h_i) is given by [17]:

$$\rho[(h_i)] = z^{-1} \exp\{-\beta\mathscr{H}[(h_i)]\} \tag{10}$$

where the Hamiltonian in the absence of the external field

$$\mathscr{H}[(h_i)] = 2J \sum_{i=1}^{L} |h_i - h_{i+1}| \tag{11}$$

is, up to a constant L, proportional to the length of the line dividing the system into two regions occupied by different incompressible phases (liquid and gas or up and down magnetised domains). The density profile and the density correlation function are related to the probability $p(h)$ of height h and to the joint probability $p_2(h_i, h_j)$ of heights h_i and h_j of the ith and jth columns in the following way:

$$\rho(z_i) = \sum_{h_i = z_i}^{M} p(h_i) \tag{12a}$$

$$H(i, j; z_i, z_j) = \sum_{\substack{h_i = z_i \\ h_j = z_j}}^{M} P(h_i, h_j) \tag{12b}$$

where

$$P(h_i, h_j) = p_2(h_i, h_j) - p(h_i)p(h_j). \tag{13}$$

Our present calculations are based on the results of [6] for p and p_2 in the two asymptotic cases L and M.

2.1. Case M

The expressions (3.7) of [6] and equations (12) above lead to the following form of H:

$$H(\Delta x, z_1, z_2) = \frac{1}{2(M+1)^2} \sum_{\substack{h_1 = z_1 \\ h_2 = z_2}}^{M} \cos\left(\frac{h_1}{W}\right) \cos\left(\frac{h_2}{W}\right) \sum_{n=1}^{2M+1} \left[\cos\left(\frac{n\Delta h}{W}\right) + (-1)^{n+1} \cos\left(\frac{n(h_1 + h_2)}{W}\right)\right] \left(\frac{\lambda_n}{\lambda_1}\right)^{\Delta x} - \rho(z_1)\rho(z_2) \tag{14}$$

where (see (3.5) in [6])

$$\lambda_n = \frac{\sinh(2K)}{\cosh(2K) - \cos(n/W)} \tag{15}$$

with

$$K = \beta J \tag{16}$$

and W is given in (2c).

The cases $\Delta x \ll M^2$ and $\Delta x / M^2 \gg 1$ will be considered separately.

2.1.1. Case $\Delta x \ll M^2$. Let us consider the function $f(p) = (\lambda_n/\lambda_1)^{\Delta x}$ where

$$p = \cos(n/W) - 1 \tag{17}$$

and expand f in a Taylor series about $p = 0$:

$$f(p) = \sum_{k=0}^{\infty} \frac{f^{(k)}(0)(2p)^k}{k!2^k}. \tag{18}$$

Using the relation

$$\sum_{n=1}^{2M+1} [2(\cos(n/W) - 1)]^m \cos(nk/W) g(n) = \Delta_2^m \sum_{n=1}^{2M+1} \cos(nk/W) g(n) \tag{19}$$

where

$$\Delta_2 \tilde{g}(k) = \tilde{g}(k+1) + \tilde{g}(k-1) - 2\tilde{g}(k) \tag{20}$$

and

$$\Delta_2^n \tilde{g}(k) = \Delta_2(\Delta_2^{n-1} \tilde{g}(k)) \tag{21}$$

we obtain

$$H(\Delta x, z_1, z_2) = \sum_{\substack{h_1 = z_1 \\ h_2 = z_2}}^{M} \cos(h_1/W) \cos(h_2/W) \sum_{l=0} \frac{f^{(l)}(0)}{l!2^l} \Delta_2^l \sum_{n=1}^{2M+1} \{\cos(n\Delta h/W)$$
$$+ (-1)^{n+1} \cos[(n/W)(h_1 + h_2)]\} - \rho(z_1)\rho(z_2). \tag{22}$$

The following relations:

$$\sum_{n=1}^{2M+1} \{\cos(n\Delta h/W) + (-1)^{n+1} \cos[(n/W)(h_1 + h_2)]\} = 2(M+1)\delta^{\mathrm{Kr}}(\Delta h) \tag{23}$$

where δ^{Kr} denotes the Kronecker symbol, and

$$\left.\frac{\mathrm{d}f(p)}{\mathrm{d}p}\right|_{p=0} = \frac{\Delta x}{2\sinh^2 K} \tag{24}$$

enable us to rewrite (21) in the form

$$H(\Delta x, z_1, z_2) \underset{M\to\infty}{=} [2(M+1)^2]^{-1} \sum_{\substack{h_1 = z_1 \\ h_2 = z_2}}^{M} \cos(h_1/W) \cos(h_2/W) 2(M+1) \Bigg(\delta^{\mathrm{Kr}}(\Delta h)$$
$$+ \frac{\Delta x}{4\sinh^2 K} [\delta^{\mathrm{Kr}}(\Delta h + 1) + \delta^{\mathrm{Kr}}(\Delta h - 1) - 2\delta^{\mathrm{Kr}}(\Delta h)] \Bigg)$$
$$- \rho(z_1)\rho(z_2) + \mathrm{O}\left(\frac{\Delta x^2}{W^4}\right). \tag{25}$$

The expression (25) may be rewritten in the following scaling form:

$$H(\Delta x, z_1, z_2) = H_s(\Delta x^*, z_1^*, z_2^*) = \rho_s(z_{\max}^*)(1 - \Delta x^*) - \rho_s(z_1^*)\rho_s(z_2^*) + \mathrm{O}(\Delta x^*) \tag{26}$$

where the rescaled distance is given by

$$\Delta x^* = \Delta x/\xi_\perp(M) \qquad \xi_\perp = 4\sinh^2 K W^2. \tag{27}$$

Let us note that the relation between $\xi_\perp$ and W is of the form (9) because in the solid-on-solid model the effective surface tension Γ is [10]

$$\beta\Gamma = 2\sinh^2 K. \tag{28}$$

2.1.2. Case $\Delta x \gg M^2$. In this case we are interested in the behaviour of H in the asymptotic region of large Δx^*. Equation (14) involves the function

$$\left(\frac{\lambda_n}{\lambda_1}\right)^{\Delta x} \underset{M\to\infty}{=} \begin{cases} O(M)^{-l} & l \text{ arbitrary} \qquad\qquad\qquad\qquad n \sim M \\ \left\{1 - \dfrac{n^2-1}{2\beta\Gamma W^2} + O\left[\left(\dfrac{n}{W}\right)^4\right]\right\}^{2\beta\Gamma W^2 \Delta x^*} \underset{W\to\infty}{=} \exp[-(n^2-1)\Delta x^*] & n \ll M. \end{cases} \tag{29}$$

The terms with $n \sim M$ are negligible. In the case of $\Delta x^* \to \infty$ the terms with $n \geqslant 3$ in the sum (14) are also negligible. We truncate this sum on the second term and obtain

$$H_s(\Delta x^*, z_1^*, z_2^*) = \frac{1}{9\pi^2} p_s^{3/2}(z_1^*) p_s^{3/2}(z_2^*) \exp(-3\Delta x^*)[1 + O(\exp(-5\Delta x^*))]. \tag{30a}$$

The Fourier transform of H is

$$H_s(k, z_1^*, z_2^*) \underset{k\to 0}{=} \frac{2p_s^{3/2}(z_1^*) p_s^{3/2}(z_2^*)}{3(9 + k^2 \xi_\perp^2)}. \tag{30b}$$

The form of H for $\Delta x^* \to 0$ is the same as in the case of $g \neq 0$ in the capillary-wave theory [14, 15] whereas in the case of $\Delta x^* \to \infty$ it is similar but not exactly the same. This difference is an effect of the boundaries of the system. The mean displacement of the 'instantaneous' interface W is of the order of M and considerable numbers of capilllary waves are eliminated. Even in a very large system the walls affect the structure of the interface.

2.2. Case L

In this case we restrict our considerations to $H(\boldsymbol{r}_1, \boldsymbol{r}_2)$ for points $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$ far from boundaries because of the boundary condition $h_1 = h_L = 0$. Only distances $\Delta x \ll L$, for which the system is translationally invariant in a transverse direction in the asymptotic region of $L \to \infty$ [6], will be considered. The forms of the functions p and p_2 given in (3.9) of [6] lead to the expression

$$H(\Delta x, z_1, z_2) = \frac{2 \sinh K}{L} \sum_{\substack{h_1 = z_1 \\ h_2 = z_2}} \exp[-2\sinh^2 K(h_1^2 + h_2^2)/L] \frac{(a-1)^{\Delta x}}{\pi} \int_0^\pi dk \frac{\cos(k\Delta h)}{(a - \cos k)^{\Delta x}} \tag{31}$$

where

$$a = \cosh 2K. \tag{32}$$

As in the previous case we expand the function

$$f(p) = \left(\frac{a-1}{a - \cos k}\right)^\Delta$$

where $p = \cos k - 1$ about $p = 0$ and use the relations

$$\int_0^\pi dk[2(\cos k - 1)]^n \cos(kx) g(k) = \Delta_2^n \int_0^\pi dk \cos(kx) g(k) \tag{33}$$

and

$$\int_0^\pi dk \cos(kx) = 2\delta^{\mathrm{Kr}}(x). \tag{34}$$

The result is as follows:

$$H(\Delta x, z_1, z_2) = \frac{2\sinh K}{L}\sum_{n=0}^{\infty}\sum_{\substack{h_1=z_1\\h_2=z_2}}^{M}\exp[-2\sinh^2 K(h_1^2+h_2^2)/L]\frac{f^{(n)}(0)}{n!2^n}\Delta_2^n\delta^{\mathrm{Kr}}(\Delta h). \quad (35)$$

Using the form (24) of $f(p)|_{p=0}$ and the form (3) of the density profile (see (4.4) in [6]) we obtain in the asymptotic region of $L\to\infty$ the same form as in the case M for small Δx^*, namely (26) but with the transverse length scaled according to

$$\Delta x^* = \Delta x/\xi_\perp(L) \qquad \xi_\perp = L. \quad (36)$$

In this case the interface thickness W is given by (2) and so the relation between W and $\xi_\perp$ is also of the form (9).

3. Conclusions

The exact results obtained in the case of $g=0$ in the finite two-dimensional solid-on-solid system in the asymptotic regions of $L=\infty$ and M large but finite or $M=\infty$ and L large show that H depends on L and/or M only via length scales. In the systems considered the Weeks [9] scaling hypothesis is verified. The relation between transverse $\xi_\perp$ and longitudinal (W) characteristic lengths has the same form (9) in both cases and in the case of $g\neq 0$ in the capillary-wave model. In the case of finite L in which $\xi_\perp = L$ the relation (9) is valid in the capillary-wave model as well [15]. Thus this relation seems to be the universal feature of the interface, independent of the external conditions and details of the interparticle potential.

The forms of the rescaled functions $\rho_s(z^*)$ and $H_s(\Delta x^*, z_1^*, z_2^*)$ depend on how the interface is localised and are not universal. In the cases of $g\neq 0$ and finite L the forms of ρ_s and H_s are the same but differ from the corresponding functions in the case of finite M.

In given external conditions, according to the scaling hypothesis, $\xi_\perp$ and W stand for the only relevant length in the interface zone. If the scaling hypothesis is correct, the results obtained in the solid-on-solid model, in which the fluctuations over the range of bulk correlation length ξ_b are neglected, should apply to more realistic models (with short-range interparticle interactions) in which such fluctuations are taken into account. The density profile has indeed the same form in solid-on-solid and in lattice-gas models (see (3)). It is plausible that the same property exhibits the density correlation function and our results are not limited to this simple model if $T \ll T_c$. In the high-temperature region (i.e. for $T\to T_c$) both the interface scaling hypothesis [9] and the solid-on-solid model (as an approximation to a lattice gas) are not correct because ξ_b becomes important.

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