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The dependence on external field of the correlation functions and susceptibilities of the one-dimensional SOS interface†

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Abstract. A numerical study of the SOS interface in two dimensions extends the asymptotic analysis of van Leeuwen and Hilhorst. Global properties, one-point functions, and two-point correlations computed earlier, including the direct correlation function and the susceptibilities, are parametrised and their dependence on the external field is analysed in detail. Intrinsic properties of the interface, including the new longitudinal correlation length, are discussed.

1. Introduction

The statistical theory of the interfacial phenomena faces a well known difficulty posed by the fluctuations of the interface (see e.g. Rowlinson and Widom 1982, Abraham 1982, van Leeuwen and Hilhorst 1981, Jasnow *et al* 1982; for a recent review see Binder (1983)). A system separates into two phases owing to an external (e.g. gravitational) field which localises the position of the interface in space. The field will also damp the fluctuations of the interface about this position. Hence any quantity such as the density profile depends on the amplitude of the external potential and immediately the question arises as to which quantities may be accepted as *intrinsic* properties of the interface. The fluctuations of the interface are particularly strong in two-dimensional ($d = 2$) systems with one-dimensional interfaces ($d_s = 1$). Here we study in detail a particularly simple system, the solid-on-solid (SOS) lattice model, which replaces the interface of a lattice gas by an array of columns of occupied sites. In two dimensions this is the Temperley string (Temperley 1952) which, however, we place in an external field. Analytic and numerical results have been obtained and some asymptotic analysis for small external field is also available (van Leeuwen and Hilhorst 1981). We use the method of the transfer matrix which is constructed and diagonalised numerically; for the nearest-neighbour interactions this is a straightforward and accurate technique. In § 2 we give the working equations, and give the results for the global quantities of the system. In § 3 we give the results of the scaling of distances for the z -dependent local susceptibility and for the two-point density-density correlation function $H(1, 2)$. Then we parametrise its inverse, the direct correlation function $C(1, 2)$. Also in § 3 we demonstrate the existence of a longitudinal correlation length $\xi_{||}$ which in the limit of the vanishing external field becomes identical to the longitudinal correlation length recently discovered by Ciach (1985) for the zero field case.

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The remarkably transparent structure of the direct correlation function matrix $C(z_1, z_2)$ is discussed.

2. The transfer matrix and asymptotic results for the sos model

The sos model of a strip of height M and horizontal length L is a collection of L columns ($i = 1, 2, \dots, L$) of heights $0 \leq h_i \leq M$ interacting through a nearest-neighbour interaction, with the partition function

$$Z = \sum_{h_1} \dots \sum_{h_L} \prod_{i=1}^L \exp[-\beta\epsilon|h_i - h_{i+1}| - \beta H^{\text{ext}}(i)] \quad (2.1)$$

where $\beta\epsilon = 2\beta J = 2K > 0$ and the periodic boundary conditions are assumed in the horizontal direction along the x coordinate. We take $x = \text{integer}$, $0 \leq x \leq L$. Let the external potential $H^{\text{ext}}(i)$ result from the gravitational potential

$$\beta V^{\text{ext}}(z, x) = \beta mg(z - z_0) \quad (2.2)$$

acting on each filled site of a column; thus

$$\beta H^{\text{ext}}(i) = G(h_i - h_0)^2 \quad (2.3)$$

where $h_0 = z_0 - \frac{1}{2}$, $G = \beta mg/2$ and the energy zero has been shifted (by LGh_0^2). This adjustment ensures that there is no change in the free energy if the interface is shifted vertically by an infinitesimal amount

$$\delta \ln Z / \delta h_0 = 0. \quad (2.4)$$

The transfer matrix has been used before (van Leeuwen and Hilhorst 1981, Dudowicz 1984, Dudowicz and Stecki 1980, 1985, Stecki 1984); for our discussion here the asymptotic result (van Leeuwen and Hilhorst 1981) is especially important. We define a symmetric (column-column) transfer matrix by

$$T_{mn} = \exp[-G(n-1-h_0)^2/2] \exp(-2K|m-n|) \exp[-G(m-1-h_0)^2/2] \quad (2.5)$$

of dimension $M+1$ which is diagonalised numerically, and its eigenvalues $\lambda_1 > \lambda_2 > \dots$ and corresponding eigenvectors $x^{(1)}, x^{(2)}, \dots$, are found to be

$$T x^{(I)} = \lambda_I x^{(I)}, \quad \lambda_1 > \lambda_2 > \dots, \quad I = 1, 2, \dots, M+1. \quad (2.6)$$

We take $L \rightarrow \infty$; M finite. A finite M is equivalent to two impenetrable walls at $z = 0$ and $z = M+1$ limiting the fluctuations of the interface. Therefore for each fixed value of the external-field amplitude G we increase the 'vertical' size M until we are satisfied that the interface is pinned by G and not by the finite size M . All the quantities we need can be expressed in terms of the eigenvalues and eigenvectors; the density profile

$$\rho(z) = \sum_{h \geq z} p(h) \quad (2.7)$$

and probability of a height h

$$p(h) = [x_h^{(1)}]^2. \quad (2.8)$$

In the asymptotic analysis of van Leeuwen and Hilhorst (1981) the finite height differences were replaced by derivatives and the differential equation for the harmonic oscillator was obtained, in the variable

$$y = G^{1/4}(2S)^{1/2}(h - h_0), \quad S \equiv \sinh K. \quad (2.9)$$

This analysis can be applied to several of the quantities we consider and invariably the first term agrees perfectly with the coefficient extracted from the numerical data. Since the accuracy of the data obtained with the transfer matrix method is limited only by the performance of the computer in the diagonalisation procedure, the extraction of the coefficients is easy and reliable.

Figure 1 shows the convergence of several eigenvalues towards $\lambda_{\max}(G=0) = \coth K$ in perfect agreement with the prediction of van Leeuwen and Hilhorst (1981). Figure 2 shows the density profiles for various fields in the same range, scaled with the variable y defined by (2.9); clearly $\rho(y)$ falls on a common curve (erfc(y) in fact), with a derivative $\rho'(y=0) = (1/\sqrt{\pi})$. Another important one-point function is a local susceptibility

$$\tilde{\chi}(z) \equiv \chi(\mathbf{r}_1) = \frac{\delta\rho(1)}{\delta(-\beta V^{\text{ext}})} = \sum_{(2)} \frac{\delta\rho(1)}{\delta(-\beta V^{\text{ext}}(2))} \tag{2.10}$$

which also arises in the sum rules for the two-point density-density correlation function $\tilde{H}(z_1, z_2; k)$ discussed in § 3. In (2.10) it is understood that at each field point '2' the increment of $-\beta V^{\text{ext}}(2)$ is the same. Summing over \mathbf{r}_1 one obtains the ordinary (total) susceptibility

$$\chi_T \equiv \sum_z \tilde{\chi}(z) = \frac{1}{L} \sum_{(1)} \chi(1) = \frac{1}{L} \frac{\partial^2 \ln Z}{\partial(-\beta V^{\text{ext}})^2} \tag{2.11}$$

where again the increment of V^{ext} must be the same at all lattice points. Incidentally this is different from

$$\chi_G \equiv \frac{1}{L} \frac{\partial^2 \ln Z}{\partial G^2}, \quad G = \beta mg/2, \tag{2.12}$$

with Z given by (2.1)-(2.3), which is

$$\chi_G = \overline{(h_1 - h_0)^2} - \overline{(h_1 - h_0)}^2 + \frac{1}{L} \sum_i \sum_{j \neq i} [\overline{(h_i - h_0)(h_j - h_0)} - \overline{(h_i - h_0)}\overline{(h_j - h_0)}]. \tag{2.13}$$

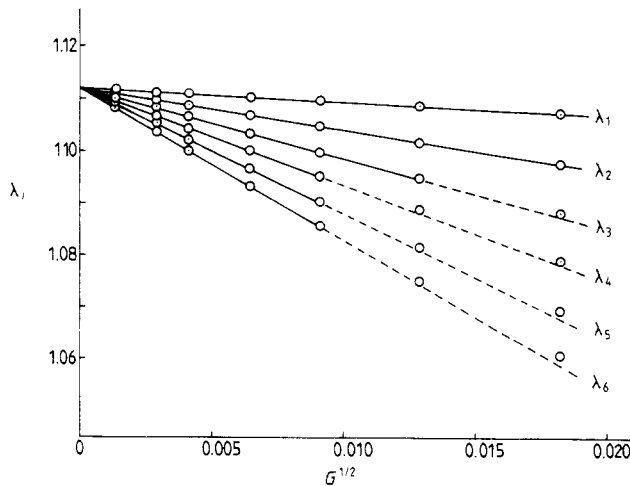


Figure 1. The eigenvalues $\lambda_i (i = 1-6)$ of the transfer matrix extrapolated to $G = 0$ converge towards $\lambda_{\max}(G = 0) = \coth K = 1.111\ 879\ 409\ 30$. Data were obtained for $35 \leq M \leq 129$, in the range of $1.666\ 66 \times 10^{-6} \leq G \leq 3.333\ 33 \times 10^{-4}$ at $T = 0.3 T_c$, $2K = 2\beta J = 2.937\ 912$.

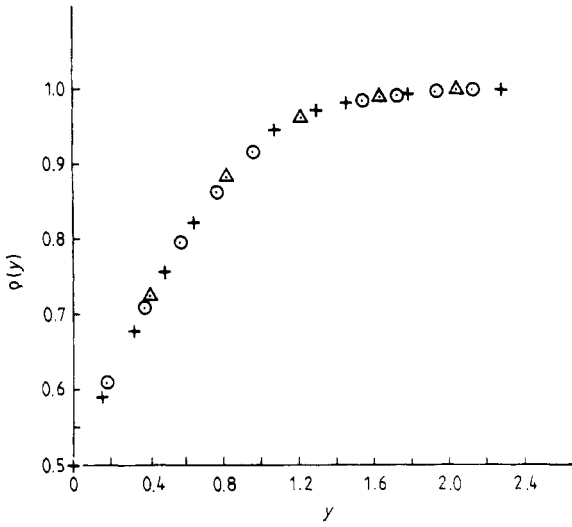


Figure 2. The density $\rho(y)$ against $y = (2 \sinh K\sqrt{G})^{1/2} h_1$ at $T = 0.3T_c$, $2K = 2\beta J = 2.937912$. Data points: +, ($G = 0.41666 \times 10^{-4}$), \odot , ($G = 0.083333 \times 10^{-4}$), and Δ , ($G = 1.66666 \times 10^{-3}$), fall on a common curve.

The local z -dependent susceptibility scales very well with the variable y and

$$\chi(z) = \chi(z_0 + \frac{1}{2}) \exp(-ay^2) \tag{2.14}$$

with

$$a = 1 + a_1\sqrt{G} + \dots, \tag{2.15}$$

$$\chi(z_0 + \frac{1}{2}) = (S/2\pi)^{1/2} G^{-3/4} + b_1 2^{-3/4} G^{-1/4} + b_2 2^{-3/4} G^{1/4} + \dots \tag{2.16}$$

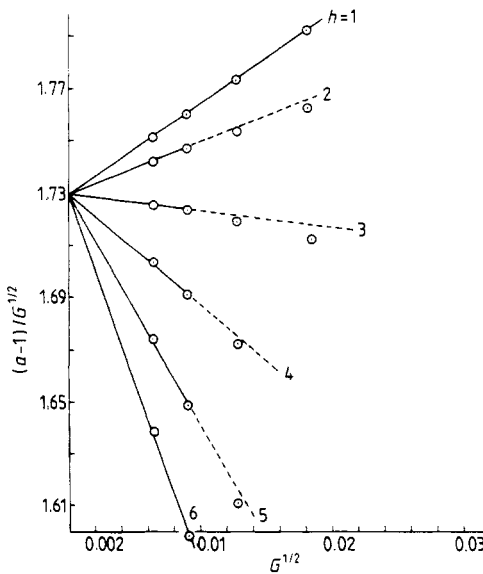


Figure 3. The coefficient a_1 determined from (2.14)-(2.15) for $T = 0.3T_c$, $2K = 2\beta J = 2.937912$, $0.41666 \times 10^{-4} \leq G \leq 1.66666 \times 10^{-4}$, strip height $41 \leq M \leq 55$. a_1 extrapolates to a common value $a_1 = 1.73$ at $\sqrt{G} = 0^+$.

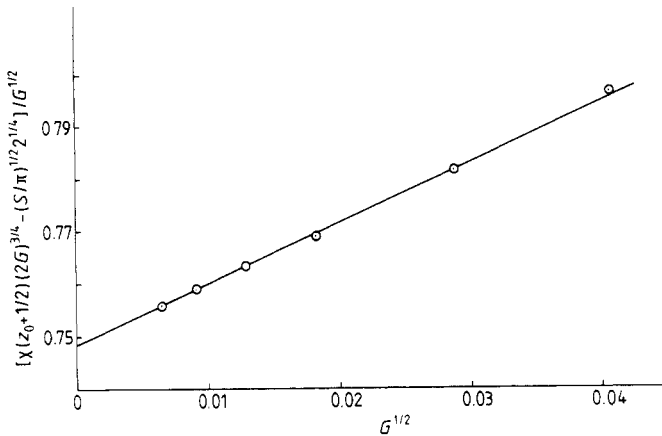


Figure 4. Test of validity of (2.16). The ordinate equals $b_1 + b_2 \sqrt{G}$; at $T = 0.3 T_c$, $2K = 2\beta J = 2.937\ 912$, $b_1 = 0.747\ 912$, $b_2 = 1.182$. Data were obtained for $29 \leq M \leq 55$, $0.416\ 66 \times 10^{-4} \leq G \leq 1.666\ 66 \times 10^{-3}$.

The local susceptibility at any given value of z diverges and figures 3 and 4 show how (2.15) and (2.16) are established. Finally we find by summing (2.14)

$$\chi_T = 2/G + wG^{-1/2} + \dots \tag{2.17}$$

with w a very small number at low temperatures (at $T = 0.3 T_c(d = 2)$ for which $2K = 2\beta J = 2.938$, $w = 5.55 \times 10^{-5}$). No $G^{-3/4}$ power could be detected at our values of G . Thus the one-point functions appear to follow a universal behaviour, and are scaled by the van Leeuwen variable y , defined in equation (2.9). The susceptibilities diverge as G^{-1} or $G^{-3/4}$.

3. The two-point correlation functions

The density-density correlation function $H = \langle \delta\rho(1)\delta\rho(2) \rangle$ or

$$H(1, 2) = \delta^{Kr}(1, 2)\rho_1(1) + \rho_2(1, 2) - \rho_1(1)\rho_1(2) \tag{3.1}$$

is a function of three variables $z_1, z_2, \Delta x = r_{12}^+$ and its Fourier transform can be computed directly for $L \rightarrow \infty$ from eigenvalues and eigenvectors of T :

$$\hat{H}(z_1, z_2; k_\perp) = \sum_{\text{all } x} \exp(ik_\perp \Delta x) H(z_1, z_2, \Delta x) \tag{3.2}$$

$$\begin{aligned} &= H(\Delta x = 0) + \sum_{I \geq 2} C(I) f_I(k) \\ &= \sum_{I \geq 2} C(I) [1 + f_I(k)] \end{aligned} \tag{3.3}$$

with

$$C(I) = C'(z_1, I) C'(z_2, I), \tag{3.4}$$

$$C'(z, I) = \sum_{n=1+z}^{M+1} x_n^{(1)} x_n^{(I)}, \tag{3.5}$$

$$1 + f_I(k) = \frac{(1 - r_I)(1 + r_I)}{(1 - r_I)^2 + 2r_I(1 - \cos k)}. \tag{3.6}$$

At a given amplitude of the external field, G , \tilde{H} is a smooth function of k and for each value of k , including $k = 0$, peaked about $z_1 = z_2 = z_0 + \frac{1}{2}$. Introducing the variables y_1 and y_2 after equation (2.9), we find a parametrisation of \tilde{H} in terms of the variables

$$Y = \frac{1}{2}(y_1 + y_2), \quad y_{12} = y_2 - y_1, \tag{3.7}$$

of the following form:

$$\tilde{H}(Y, y_{12}) = \tilde{H}(0, 0) \exp(-\alpha y_{12}^2) \exp(-A_0 Y^2 - A_2 Y^4 - A_4 Y^6). \tag{3.8}$$

As $\sqrt{G} \rightarrow 0$, we find

$$\tilde{H}(0, 0) = (S/\sqrt{G})(H^* + H_1\sqrt{G} + \dots), \tag{3.9}$$

$$\alpha = \alpha_0 + \alpha_1(\Delta z)\sqrt{G} + \dots, \tag{3.10}$$

$$A_0 = A_{00} + A_{01}(\Delta z)\sqrt{G} + \dots, \tag{3.11}$$

$$A_2 = A_{20} + A_{21}(\Delta z)\sqrt{G} + \dots, \tag{3.12}$$

$$A_4 = A_{40} + A_{41}(\Delta z)\sqrt{G} + \dots, \tag{3.13}$$

where the coefficients $\alpha_1, A_{01}, A_{21}, A_{41}$ depend on $\Delta z = |z_2 - z_1|$. Figures 5-7 show how the parameters $H^*, H_1, \alpha_0, A_{00}$ were established. A_{20} and A_{40} are much smaller, e.g. at $T = 0.3 T_c, A_{20}/A_{00} = -0.0232, A_{40}/A_{00} = -0.00093$. This parametrisation is not very satisfactory because the dependence on \sqrt{G} is rather strong and moreover the coefficients depend on Δz . As we describe below, a similar parametrisation of C is much easier and much more satisfactory. Nevertheless a numerical diagonalisation of the matrix (3.8) produces λ_{\max} which agrees within 10% with λ_{\max} of the exact matrix \tilde{H} .

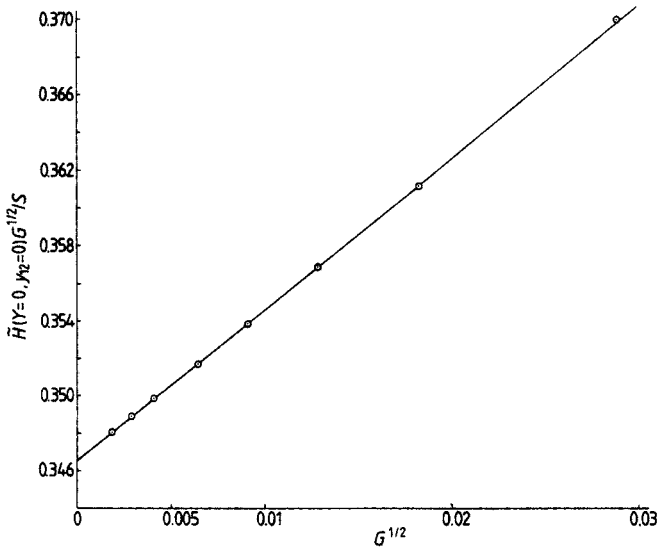


Figure 5. Variation of the largest element of the \tilde{H} matrix with \sqrt{G} . $\tilde{H}(Y=0, y_{12}=0)\sqrt{G}/\sinh K$ varies linearly with \sqrt{G} . At $T = 0.3 T_c, 2K = 2\beta J = 2.937912$, the intercept $H^* = 0.3465$, the slope $H_1 = 0.7826$. Data were obtained for $29 \leq M \leq 55, 0.41666 \times 10^{-4} \leq G \leq 0.333333 \times 10^{-3}$.

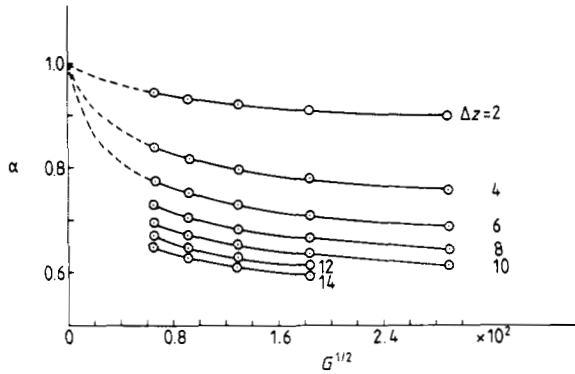


Figure 6. The parameter α (from (3.8)) computed as $-y_{12}^{-2} \ln|\tilde{H}(Y=0, y_{12})/\tilde{H}(0, 0)|$ plotted against \sqrt{G} . Curves are labelled with values of $\Delta z = |z_2 - z_1|$ and appear to converge to a common α value at $\sqrt{G} = 0$. Data were obtained for the same range as in figures 1-5.

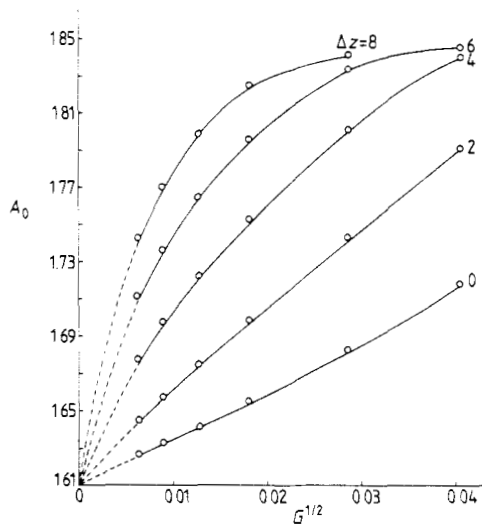


Figure 7. The coefficient A_0 (see (3.8)) determined from finite differences of the function $-y_{12}^{-2} \ln|\tilde{H}(Y, y_{12})/\tilde{H}(Y=0, y_{12})|$ and plotted against \sqrt{G} . The intercept $A_{00} = 1.6121$ at $T = 0.3 T_c$ appears to be common to all y_{12} . Curves are labelled with values of $\Delta z = |z_2 - z_1|$. Data were obtained for the same range as in figures 1-6.

The k dependence of \tilde{H} is regular and not in contradiction to the predictions of the capillary wave theory (Evans 1979, Weeks 1977, Wertheim 1976) concerning the form

$$\tilde{H} = \tilde{H}(k=0) \frac{\beta mg \Delta \rho}{\beta mg \Delta \rho + \beta \gamma k^2}, \quad G = \text{constant}, \quad (3.14)$$

but a detailed analysis of $\tilde{H}(k, G)$ remains to be carried out. Summing over z_2 we obtain the local susceptibility $\tilde{\chi}(z_1, k)$ and summing over z_1 we obtain the k -dependent total susceptibility which has been analysed. The working equation now follows directly from (3.3)-(3.6) by summing over z_1 and z_2 and changing the order of summation.

Then we found that the sum over eigenvalues ($I \geq 2$) reduces effectively to the $I = 2$ term with an excellent accuracy if G is not too large. Rewriting (3.6) in terms of $\varphi(k) = 2(1 - \cos k) = k^2 - k^4/12 + \dots$ and $\Delta = 1 - r_2$, we find

$$\tilde{\chi}_T(k) = D(I = 2) \frac{\Delta(2 - \Delta)}{\Delta^2 + (1 - \Delta)\varphi(k)} + a_1\sqrt{G} + \dots \tag{3.15}$$

Certainly this form of $\tilde{\chi}_T(k)$ agrees fully with the predictions of the capillary wave theory. For small G we find

$$\Delta = \sqrt{G}/S - r_{22}G - r_{23}G^{2/3} - \dots, \tag{3.16}$$

$$D(I = 2) = 1/(4 S\sqrt{G}) + d_{20} + d_{21}\sqrt{G} + \dots \tag{3.17}$$

Hence the leading term follows:

$$\tilde{\chi}_T(k)/\tilde{\chi}_T(k = 0) = (1 + \xi_1^2 k^2)^{-1} \tag{3.18}$$

with $\xi_1^2 = 2S^2/2G$ which allows for the identification

$$\beta\gamma_{\text{eff}} = 2S^2. \tag{3.19}$$

Computing the derivative of $\tilde{\chi}_T(k)$ with respect to k^2 we find directly from (3.15)

$$\beta\gamma_{\text{eff}} = 2S^2 + g_1\sqrt{G} + \dots \tag{3.20}$$

This relation is shown in figure 8 taken from numerical data. It is remarkable that the field dependence should be so strong. This value, $2S^2$, does not agree with $\ln \lambda_{\text{max}} = \ln \coth K$ because it incorporates the angle dependence of the surface tension and agrees with the sos limit of the exact results of Abraham (1981), Abraham and Reed (1974) and Fisher *et al* (1982) as described by Binder (1983).

The parametrisation of \tilde{C} was remarkably straightforward. First, we recall the exact relation for the sos system in two dimensions (Stecki 1984),

$$C(z_1, z_2, \Delta x) = 0, \quad \text{for } |\Delta x| \geq 2, \tag{3.21}$$

from which it follows that

$$\tilde{C}(z_1, z_2, k_\perp) = C_0 + 2C_1 \cos k = C_0 + 2C_1 - C_1\varphi(k). \tag{3.22}$$

The two matrices C_0 and C_1 refer to $\Delta x = 0$ and $\Delta x = \mp 1$, respectively. Introducing the variable Z by $2Z = z_1 + z_2$ and $\Delta z = |z_2 - z_1|$ we find that all three matrices scale their Z dependence with the external field according to the variable introduced by van Leeuwen and Hilhorst (1981), equation (2.9). However, the variable Δz refuses to be scaled in the same manner. Hence

$$\tilde{C}(z_1, z_2) = G^{-1/4} M \exp(A_0 Y^2 + A_2 Y^4 + A_4 Y^6) \tag{3.23}$$

where $A_0 = 1, A_2 = A_4 = 0$ for $G \rightarrow 0^+$, and the new matrix M depends only weakly on the external field

$$M = tu^{|\Delta z|} + D. \tag{3.24}$$

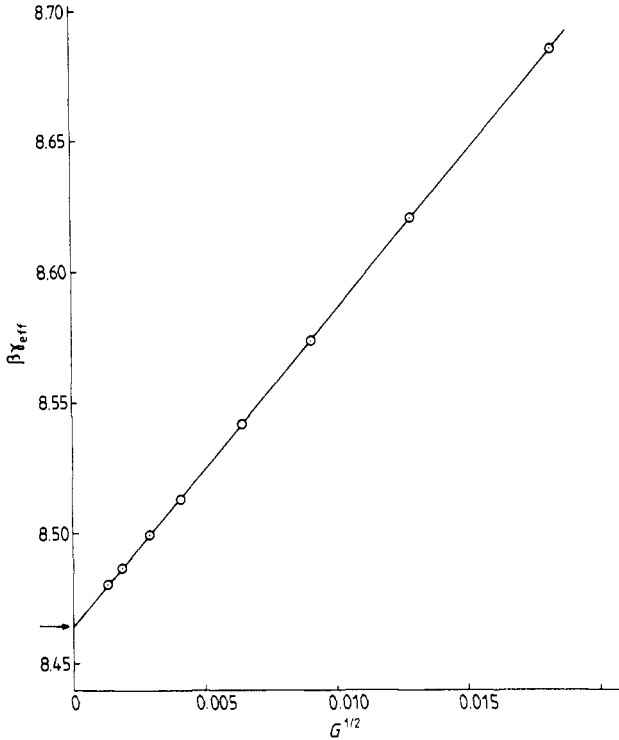


Figure 8. Variation with \sqrt{G} of the effective surface tension, $\beta\gamma_{\text{eff}}$, computed from (3.15). The arrow indicates the value $2 \sinh^2 K = 8.46683316$ which is the value of $\beta\gamma_{\text{eff}}$ for $\sqrt{G} = 0$. The slope $g_1 = 11.767367$. The data were obtained for $35 \leq M \leq 129$ and $1.6666 \times 10^{-6} \leq G \leq 3.3333 \times 10^{-4}$.

Here D is a tridiagonal (symmetric) matrix, $D = 0$ unless $\Delta z = 0, 1$, $D = D_0^{(\nu)} \delta^{Kr}(\Delta z, 0) + D_1^{(\nu)} \delta^{Kr}(\Delta z, 1)$, where the index ν distinguishes between C_0, C_1 and $\tilde{C}(k=0) = C_0 + 2C_1$; similarly the number t is different in these cases.

Hence we find a remarkably simple structure; we recall that a matrix of the form $u^{|\Delta z|}$ is the inverse of a tridiagonal matrix, thus $M = D + (D')^{-1}$, with

$$D' = t^{-1} \left[\delta^{Kr}(\Delta z, 0) \frac{1+u^2}{1-u^2} + \delta^{Kr}(\Delta z, 1) \left(u - \frac{1}{u} \right)^{-1} \right]. \tag{3.25}$$

The inverse of C is H and the inverse of M is $D'(U + DD')^{-1}$; DD' is a pentadiagonal matrix and M^{-1} will not have a simple structure immediately apparent. Figure 9 illustrates equation (3.23) and demonstrates how A_0 tends to 1, and how the slope of $A_0(\sqrt{G})$ depends on $|\Delta z|$. A_2 and A_4 (not plotted) are negligible, certainly so at $\sqrt{G} < 0.05$, and tend to zero as \sqrt{G} and as G , respectively. Figure 10 shows the determination of the longitudinal correlation length ($B = 1/\xi_{\parallel}$, $u = e^{-B}$) by plotting the ratios of C for $Y = 0$ or $Y = 0.5$. This new correlation length seems to be an intrinsic quantity describing the temperature-dependent structure of the interface. It appears to have a limit for $\sqrt{G} \rightarrow 0$, common to even and odd values of $|\Delta z|$ and common to all three matrices C_0, C_1 and $\tilde{C}(k=0)$. Moreover, the numerical value agrees very well with the analytic result recently obtained by Ciach (1985) who discovered the

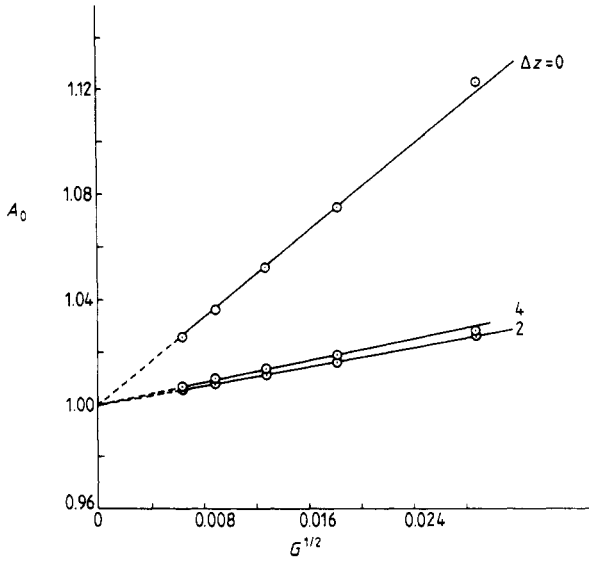


Figure 9. The coefficient A_0 in (3.23) computed from $\tilde{C}(\Delta z, Y) = \tilde{C}(\Delta z, 0) \exp(A_0 Y^2)$, plotted against \sqrt{G} . Curves are labelled with value of Δz . The range of G parameters is the same as in previous figures. A_0 appears to vary linearly with a common intercept $A_0 = 1$. Scaling of \tilde{C} with the variable Y is confirmed.

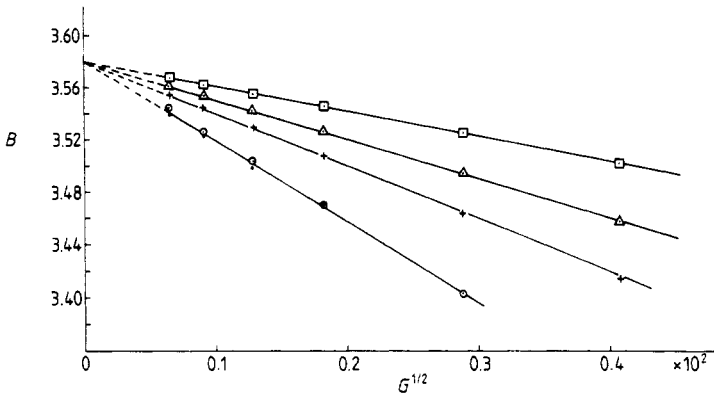


Figure 10. The inverse of the new longitudinal correlation length $B = 1/\xi_{||}$ determined from ratios of $\tilde{C}(\Delta z, Y=0)$ with $\Delta z = 0, 1$ excluded. The linear variation with \sqrt{G} and a common value of $u = e^{-B}$ at $\sqrt{G} = 0^+$ are apparent. Data are for the same range as previous figures. The zero field value $u(0) = 0.27908$ gives $B(0) = 3.5784$; the common intercept agrees very well. \square , from the ratios $C(3, 0)/C(1, 0)$ (matrix C_1 only); Δ , from the ratios $C(3, 0)/C(2, 0)$ (all three matrices C); +, from the ratios $C(4, 0)/C(2, 0)$ (all three matrices C); \odot , \bullet , from the ratios $C(5, 0)/C(3, 0)$ (\odot , matrix C_0 ; \bullet , matrix C_1).

existence of a longitudinal correlation length in finite SOS systems at zero field. According to Ciach (1985), B is a solution of $\cosh B = D^*$, with $D^* = 2 \cosh 2K - 1$. Our extrapolated values agree very well with this expression. We note that this correlation length, $\xi_{||} = -(\ln u)^{-1}$, governs the decay of \tilde{C} with increasing $|\Delta z|$, as $u^{|\Delta z|}$, and is not immediately related to the density profile nor to the scaling lengths found by Abraham (1981). $\xi_{||}$ appears to be a genuine intrinsic quantity either obtained by

$\sqrt{G} \rightarrow 0$ in surfaces pinned by G or by $M \rightarrow \infty$, $L \rightarrow \infty$ in surfaces at $G = 0$ pinned by walls. Only the free energy or $\ln \lambda_{\max}$ and $\beta\gamma_{\text{eff}} = \xi_{\perp}^2 (2G)$ appear to share this property.

Figure 11 illustrates determination of the number $\tilde{i} (k = 0)$ for the matrix $\tilde{C} (k = 0) = C_0 + 2C_1$; we find $\tilde{i} (k = 0) = t_0 + 2t_1$, $t_1 = t_0/2$ and the extrapolations made separately for C_0 and C_1 are very similar. $D_0(k = 0) = D_0^{(0)} + 2D_0^{(1)}$ and $D_1^{(0)}$ are also shown.

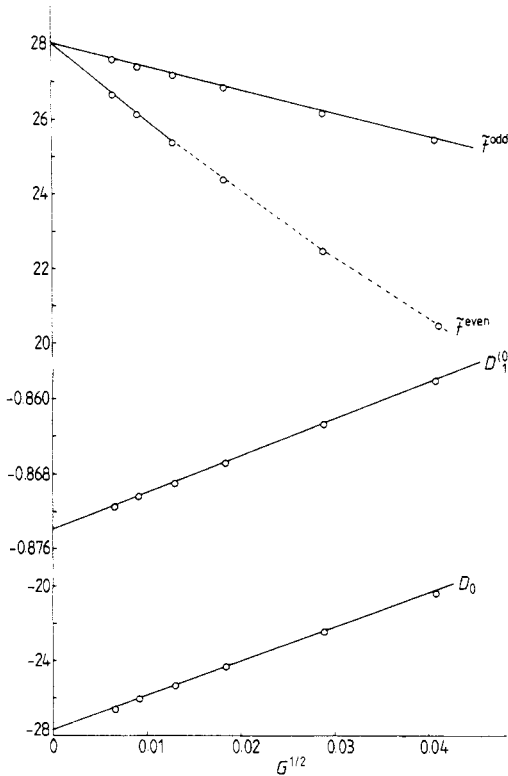


Figure 11. Parameters in the expression (3.24) for the matrix M related to $\tilde{C} (k = 0) = C_0 + 2C_1$ by (3.23); \tilde{i} from even and from odd Δz values converges to $\tilde{i} (\sqrt{G} = 0) = 27.9741$; for $\Delta z = 0$, $D_0 = D_0^{(0)} + 2D_0^{(1)} = -27.6226$; for $\Delta z = 1$, $D_1^{(0)} = -0.87397$, $D_1^{(1)} = 0$. All data are at $T = 0.3T_c$, for the range of \sqrt{G} as in previous figures.

4. Discussion

The motivation for this work has been provided by the non-analytic behaviour near $G = 0^+$ in the gravitational potential, found by van Leeuwen and Hilhorst (1981), and later for the two-point functions H and C (Stecki and Dudowicz 1984). An extension of the asymptotic analysis of van Leeuwen and Hilhorst (1981) to the two-point functions has not been made and in any case the direct correlation function would not be expressed simply; hence we had to resort to numerical computation of all the quantities. An additional bonus was a possibility of obtaining sometimes several coefficients of the successive powers of $G^{1/2}$ whereas analytical results would be limited to leading terms, if indeed they would have been obtained at all.

First of all we have confirmed in detail the ideas of van Leeuwen and Hilhorst (1981) according to which the one-point functions such as the dominant eigenvector, height probability and the density profile should scale with the scaling length y given by equation (2.9). We have found a common density profile in the variable y and we have extended this scaling to the local susceptibility. Thus we find universal behaviour for these one-point functions. The two-point function H , the density-density correlation function, scales with the variables y_1 and y_2 in the combination $Y = (y_1 + y_2)/2$, and, less satisfactorily, apparently also with the variable $y_{12} = y_2 - y_1$; in the transverse direction the decay of H is governed by the well known capillary length $\xi_{\perp}^2 = \beta\gamma/\beta mg\Delta\rho$, and the only new information we might add is that the effective surface tension depends linearly on $G^{1/2}$ with a large coefficient. Hence the external field enters into the k dependence of the Fourier transform \tilde{H} or χ quite differently from the z dependence. The existence of a longitudinal correlation length in H was not detected with the simple means we used. The inverse of H , the direct correlation function C , scales with the van Leeuwen variables only in its Y dependence and then varies with Δz according to a simple exponential variation with a longitudinal correlation length. The latter was found to be in excellent agreement with values predicted from analytical results of Ciach (1985) obtained for a finite large strip in zero field and for another two-point function which can be related to C .

Several qualitative features of H and C in the sos system were already noted by us earlier; thus we noted that $H = 0$ identically for any distance in either homogeneous sos phase with a Gaussian-like peak in the middle of the interface where obviously the density fluctuations are the largest; conversely, C does not exist in either 'homogeneous phase' of the sos system and from reasonably small positive values in the middle of the interface C increases indefinitely as we move into either phase (i.e. if both z_1 and z_2 increase or if both decrease). For a lattice gas for which in the homogeneous phases both C and H exist and can be calculated, we found as expected that both H and C approached the expected values as z_1 and z_2 were moved out of the interface zone, but in the case of C this approach was not monotonic (Stecki and Dudowicz 1985a, b). This qualitative picture points out special surface contributions to susceptibilities and H and C , which do not follow from these properties in either homogeneous phase. It also seems clear that, the problem being anisotropic, there might be *a priori* two correlation lengths (far away from a critical point which does not exist in the sos system in any case). So far the transverse correlation length has been known as such since time immemorial but the longitudinal correlation length (as distinct from scaling lengths) proved rather elusive, both theoretically and experimentally in real systems. We hope that the longitudinal correlation length we find here will also be found in other cases. Finally, it is not surprising for a one-dimensional interface that all the quantities depend so strongly on $G^{1/2}$; what is then interesting is that at least some of the quantities exist in the limit of vanishing external field. The non-analyticity is displayed explicitly and, if the leading term is extracted, often a simple polynomial in \sqrt{G} results.

References

- Abraham D B 1981 *Phys. Rev. Lett.* **47** 545
 — 1982 *Phys. Rev. B* **25** 4922
 Abraham D B and Reed P 1974 *Phys. Rev. Lett.* **33** 377

- Binder K 1983 *Phase Transitions and Critical Phenomena* vol 8, ed C Domb and M S Green (New York: Academic) p 2
- Ciach A 1986 *Phys. Rev. B* to be published
- Dudowicz J 1984 *Acta Phys. Pol. A* **66** 17
- Dudowicz J and Stecki J 1980 *Paper presented at the First Statistical Physics Seminar, Warsaw*
— 1985 *J. Phys. A: Math. Gen.* **18** 3205
- Evans R 1979 *Adv. Phys.* **28** 143
- Fisher M P A, Fisher D S and Weeks J D 1982 *Phys. Rev. Lett.* **48** 368
- Jasnow D, Pant B B and Ohta T 1982 *Phys. Rev. A* **26** 3532
- Rowlinson J S and Widom B 1982 *Molecular Theory of Capillarity* (Oxford: Clarendon)
- Stecki J 1984 *Proc. R. Soc. A* **394** 279
- Stecki J and Dudowicz J 1984 *J. Phys. A: Math. Gen.* **17** L497
— 1985a *Proc. R. Soc. A* **400** 263-87
— 1985b *Fluid Interfacial Phenomena* ed C A Croxton (New York: Wiley) ch 14
- Temperley H N V 1952 *Proc. Camb. Phil. Soc.* **48** 683
- van Leeuwen J M J and Hilhorst H J 1981 *Physica* **107A** 319
- Weeks J D 1977 *J. Chem. Phys.* **67** 3106
- Wertheim M S 1976 *J. Chem. Phys.* **65** 2377