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Asymptotic behaviour of correlation functions and the interfacial tension in the two-dimensional SOS model of an interface in zero external field

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Abstract. The modified direct correlation functions C_{cond} and C_{sym} are studied for a two-dimensional SOS system ($M \times \infty$) in a zero external field $G \equiv 0$. The asymptotic limit $W \to \infty$ of the interface width $W = (M+1)/\pi$ is considered in particular, also in connection with the Yvon-Triezenberg-Zwanzig (YTZ) formula for the interfacial tension Γ and with its modification obtained by Ciach *et al.* The successive contributions to the interfacial tension Γ, resulting from various terms of the derived relations, are computed and discussed. In the asymptotic limit $W \to \infty$ the interfacial tensions obtained from the YTZ formula and from the Ciach formula agree with each other and with Γ calculated earlier by Evans and extrapolated to $G = 0$ by Stecki and Dudowicz.

1. Introduction

In a series of papers (Stecki 1984, Dudowicz and Stecki 1985, Stecki and Dudowicz 1986a, Ciach 1986, Stecki *et al* 1986, Ciach *et al* 1987) we have studied the structure of the fluctuating interface between two coexisting phases in two dimensions, for systems with model Hamiltonians such as the columnar (solid-on-solid) model (see, e.g., van Leeuwen and Hilhorst 1981).

In particular, we have determined the asymptotic behaviour of various two-point correlation functions and of the related quantities in the limit of unbounded fluctuations of the interface. This limit is reached in an infinite system for a vanishing external (e.g., gravitational) field or alternatively in a finite system with no external field (except for boundaries which ensure spatial separation of the two coexisting phases) for system sizes increasing indefinitely. In either case the width W of the interface, conventionally defined in terms of the derivative of the density profile, diverges, $W \to \infty$.

We have extracted several quantities which exist in this limit and therefore may best be called 'intrinsic' (Stecki *et al* 1986). In a recent paper (Ciach *et al* 1987) we have studied the Yvon-Triezenberg-Zwanzig equation (see, e.g., Rowlinson and Widom 1982) and its behaviour and indeed validity in the limit of vanishing external field. In particular, we found that the original equation (see equation (3.1) below) may be interpreted as defining a certain width-dependent quantity $\Gamma = \Gamma(W)$; and that its $W = \infty$ limit exists and agrees with the interfacial tension calculated by a different route. Alternatively equation (3.8) of this paper was derived quite generally by Ciach *et al* (1987) expressing directly the limiting value of $\Gamma(W)$, i.e. the true interfacial tension, in terms of the limiting values of the new 'conditional' direct correlation function C_{cond}. I have recently noted a curious feature of the new equation (3.7) of this paper, i.e. the RHS produces zero, if the order of limit and summation (integration) is reversed. This prompted a re-examination in some detail of the relations between quantities appearing in the old YTZ equation, the Ornstein–Zernike direct correlation function in particular, and the new quantities invented by Ciach (1985) appearing in the new equation (3.8). This study, for the SOS model in two dimensions, is reported here.

In particular, we study the behaviour of these quantities and of the relations between them in the asymptotic limit $W \to \infty$, for the SOS model in two dimensions. These results acquire an additional interest in view of the most recent results by Ciach (1987) who has apparently found a non-analyticity of the direct correlation function $C(k; z_1, z_2)$ about $k = 0$ in three dimensions. The derivation of the usual YTZ equation, depending as it does on the assumption of such analyticity (see, e.g., Evans (1979) for an exhaustive review), is therefore called into question.

In § 2 we derive or quote and discuss the relations between various direct correlation functions and in particular the behaviour of these relations in the limit $W = \infty$. In § 3 we report the bulk of the results obtained for the SOS model in two dimensions, and follow with a discussion in § 4. The working equations are recalled in the appendix.

2. Conditional correlation function and symmetric correlation function

The system studied is a two-dimensional SOS $(M \times \infty)$ model, $1 \leqslant z \leqslant M$, $-\infty < x < \infty$, with periodic boundary conditions in the x direction. The solid-on-solid model replaces the interface by an array of columns of occupied sites and may be considered a good approximation at low temperatures to more elaborate models of the interface.

The reason for introducing the correlation function C_{cond}, invented by Ciach (1985), stems from the divergence of the Orstein–Zernike direct correlation function (DCF) with the size(s) of the system. C_{cond} is non-singular in this limit (Ciach 1985, 1986). The relation between C_{cond} and C is known (Ciach *et al* 1987)

$$\tilde{C}_{\text{cond}}(z_1, z_2; k_\perp) = p(z_2)\tilde{C}(z_1, z_2; k_\perp) + E_{\text{cond}} \tag{2.1}$$

where E_{cond} is a correction term vanishing with increasing W (or M) and in the general case (for given M) is

$$E_{\text{cond}} = \nabla^- p(z_2) \nabla_1^- \tilde{Q}(z_1, z_2 - 1; k_\perp) \tag{2.2}$$

where $p(i)$ is the probability of height i of a single SOS column and $\tilde{\mathbf{Q}}(k_\perp)$ is the inverse matrix of the height-height correlation function $\tilde{\mathbf{P}}(k_\perp)$

$$\tilde{\mathbf{Q}}(k_\perp) = \tilde{\mathbf{P}}(k_\perp)^{-1}. \tag{2.3}$$

The hierarchy of these functions was introduced by Stecki (1984) and is described and discussed elsewhere (Stecki 1984, Ciach 1986, Stecki and Dudowicz 1986b). The gradients ∇^+, ∇^- denote

$$\nabla^+ X(i) = X(i+1) - X(i) \tag{2.4}$$

$$\nabla^- X(i) = X(i) - X(i-1) \tag{2.5}$$

and $\tilde{X}(k, z)$ is the Fourier transform of quantity $X(x, z)$. The relations (2.1) and (2.2) are valid for any value of the Fourier variable $k_\perp$, as well as for any value of Δx; however, as found by Stecki (1984) the values of C (and C_{cond} and C_{sym}) are equal to zero for any $|\Delta x| \geq 2$, so only $C(\Delta x = 0)$ and $C(\Delta x = 1)$ contribute to $\tilde{C}(k_\perp)$ in the SOS system:

$$\tilde{C}(k_\perp) = C(\Delta x = 0) + 2C(\Delta x = 1) \cos k_\perp. \tag{2.6}$$

In the limit $M \to \infty$ $(W \to \infty)$, at zero external field $G \equiv 0$, $\tilde{C}_{\text{cond}}(k_\perp)$ (or $C_{\text{cond}}(\Delta x)$) depend on one position variable $|\Delta z| = |z_2 - z_1|$ only, instead of two (z_1 and z_2 or Δz and $y = (z_1 + z_2 - M)/2$ equivalently):

$$\lim_{\substack{M\to\infty \\ (W\to\infty)}} \tilde{C}_{\text{cond}}(z_1, z_2; k_\perp) = \tilde{C}^{\infty}_{\text{cond}}(|\Delta z|; k_\perp) \tag{2.7}$$

or

$$\lim_{\substack{M\to\infty \\ (W\to\infty)}} C_{\text{cond}}(z_1, z_2; \Delta x) = C^{\infty}_{\text{cond}}(|\Delta z|; \Delta x). \tag{2.8}$$

The LHS of (2.7) or (2.8) have the known analytical form (Ciach 1986).

First we show that, at zero external field, the difference

$$D \equiv \tilde{C}_{\text{cond}}(\Delta z, y; k_\perp) - \tilde{C}^{\infty}_{\text{cond}}(|\Delta z|; k_\perp) \tag{2.9}$$

tends to zero as the reciprocal of the square of the size of the system. Figures 1 and 2 illustrate the almost linear dependence of $D(k_\perp = 0)$ against $(M+1)^{-2}$ for $\Delta z = 0, 1, 2$ and for various values of y. The deviations from linearity are slight and increase more for larger y and M, i.e. for large distances from the Gibbs dividing surface. The correction term E_{cond} defined by (2.2) tends to zero with $M \to \infty$ (or $W \to \infty$) (Ciach 1986) and figure 3 shows (based on the example of one chosen Δz) that E_{cond} behaves also as $(M+1)^{-2}$.

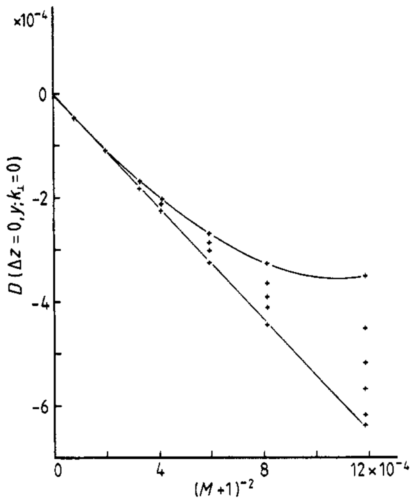

Figure 1. The difference $D(\Delta z = 0) \equiv \tilde{C}_{\text{cond}}(\Delta z = 0,\ y;\ k_\perp = 0) - \tilde{C}^{\infty}_{\text{cond}}(\Delta z = 0;\ k_\perp = 0)$ for a two-dimensional SOS $(M \times \infty)$ system at zero external field $G \equiv 0$ and at $T = 0.3\,T_c$, as a function of size M of the system ($M = 28$–70) for various values of $y \equiv (z_1 + z_2 - 2\,M_{\text{mid}})/2$, $M_{\text{mid}} = M/2$. Points for $y = 0$ lie on the straight line but for larger y we observe deviations from linearity. Points which are not connected correspond to the range $y = 3$–7 and the curve shown in the figure corrresponds to $y = 8$.

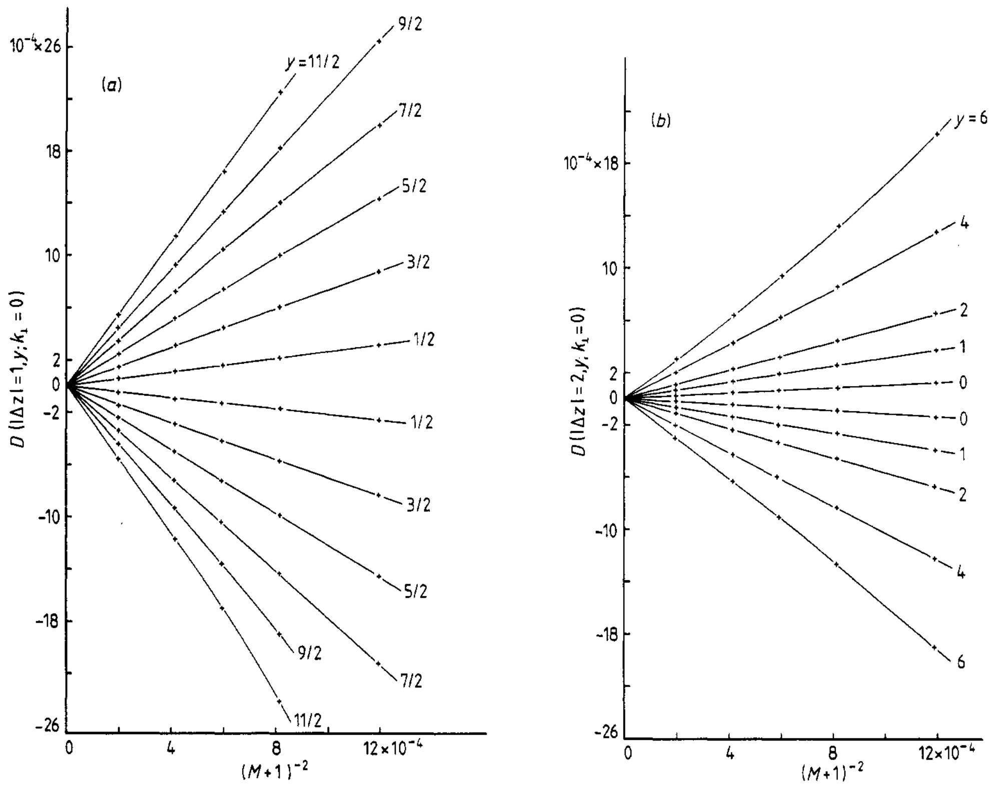

Figure 2. (a) Same as figure 1 but for $D(|\Delta z|=1)$. Positive D corresponds to $\Delta z=1$; negative D corresponds to $\Delta z=-1$. (b) Same as figure 1 but for $D(|\Delta z|=2)$. Positive D corresponds to $\Delta z=-2$; negative D corresponds to $\Delta z=2$.

The symmetric correlation function $C_{\rm sym}$ (Bedaux *et al* 1985, Ciach *et al* 1987) exhibit (contrary to $C_{\rm cond}$) a symmetry with respect to interchange of variables z_1, z_2

$$C_{\rm sym}(z_1, z_2) = C_{\rm sym}(z_2, z_1). \tag{2.10}$$

For given M we find the relation between $C_{\rm sym}$ and C:

$$C_{\rm sym}(z_1, z_2) = [p(z_1)p(z_2)]^{1/2}C(z_1, z_2) + E_{\rm sym} \tag{2.11}$$

$$\begin{aligned} E_{\rm sym} = {} & p(z_1)^{1/2}\nabla^-[p(z_2)^{1/2}]\nabla_1^- Q(z_1, z_2-1) + p(z_2)^{1/2}\nabla^-[p(z_1)^{1/2}]\nabla_2^- Q(z_1-1, z_2) \\ & + \nabla^-[p(z_1)^{1/2}]\nabla^-[p(z_2)^{1/2}]Q(z_1-1, z_2-1). \end{aligned} \tag{2.12}$$

For an infinite system $M\to\infty$ (or $W\to\infty$), the differences between z and $(z-1)$ and $\nabla[p(z)^{1/2}]$ and $\nabla p(z)/2p(z)$ can be neglected and the relation (2.11) simplifies to equation (4.8) obtained by Ciach *et al* (1987). Similarly to the correction term $E_{\rm cond}$ (see (2.2)), the correction term $E_{\rm sym}$ (2.12) also tends to zero with $M\to\infty$ (or $W\to\infty$) as $(M+1)^{-2}$.

3. The interfacial tension

The Yvon-Triezenberg-Zwanzig formula for the interfacial tension between two coexisting fluids (see, for example, Rowlinson and Widom 1982) takes the following

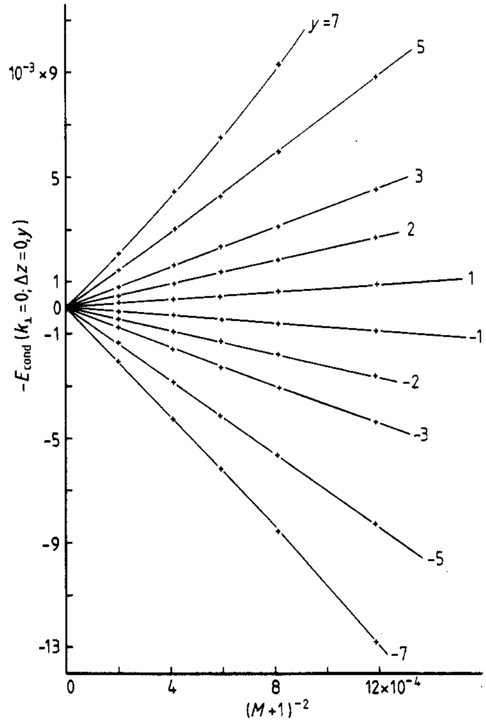

Figure 3. The correction term $-E_{\text{cond}} = \tilde{C}(k_\perp = 0; \Delta z = 0, y)p(z_2) - \tilde{C}_{\text{cond}}(k_\perp = 0; \Delta z = 0, y)$ for a two-dimensional SOS $(M \times \infty)$ system plotted against $(M+1)^{-2}$ at $T = 0.3T_c$, for various values of y, in the range $M = 28$–70.

form for the lattice system (Ciach *et al* 1987)

$$2\beta\Gamma = -\sum_{z_1} p(z_1) \sum_{z_2} p(z_2) C_2(z_1, z_2) \tag{3.1}$$

where $\beta = (kT)^{-1}$, k is the Boltzmann constant, T is the temperature, and C_2 denotes the second moment of C, defined as

$$C_2(z_1, z_2) \equiv \sum_{\Delta x} (\Delta x)^2 \, C(z_1, z_2; \Delta x) \tag{3.2}$$

$$= 2C(z_1, z_2; \Delta x = 1) \tag{3.3}$$

for the SOS system. Γ is called the effective interfacial tension because of the angle dependence of Γ in a lattice system (Binder 1983).

Also, the second moments of C_{cond} and C_{sym} are

$$C_{\text{cond2}}(z_1, z_2) = 2C_{\text{cond}}(z_1, z_2; \Delta x = 1) \tag{3.4}$$

$$C_{\text{sym2}}(z_1, z_2) = 2C_{\text{sym}}(z_1, z_2; \Delta x = 1). \tag{3.5}$$

In comparison with the original (YTZ) formula, expression (3.1) employs sums instead of integrals and probabilities $p(i) = -\nabla^+\rho(i)$ instead of derivatives $\mathrm{d}\rho(z)/\mathrm{d}z$. It cannot be applied directly to an infinite system. The remedy is to replace C_2 by C_{cond2} by using relations (2.1) and (2.2). In this way the new YTZ formula is obtained

$$\beta\Gamma(W) = -\tfrac{1}{2}\sum_{z_1} p(z_1) \sum_{z_2} C_{\text{cond2}}(z_1, z_2) + \tfrac{1}{2}\sum_{z_1} p(z_1) \sum_{z_2} \nabla^- p(z_2) \nabla_1^- Q_2(z_1, z_2 - 1) \tag{3.6}$$

where Q_2 is the second moment of Q.

For W sufficiently large, the contribution of the second term in (3.6) vanishes and we have

$$\beta\Gamma(W) = -\tfrac{1}{2}\sum_{z_1} p(z_1) \sum_{z_2} C_{\text{cond}2}(z_1, z_2;\ W). \tag{3.7}$$

If now $W \to \infty$, (3.7) takes the form containing the asymptotic limit $C^{\infty}_{\text{cond}2}$ (Ciach *et al* 1987)

$$\beta\Gamma(W=\infty) = -\tfrac{1}{2}\sum_{\Delta z} C^{\infty}_{\text{cond}2}(|\Delta z|). \tag{3.8}$$

The summation on the RHS of (3.8) with the analytic form of $C^{\infty}_{\text{cond}2}$ (Ciach 1985, 1986) produces $2\sinh^2 K \equiv 2s^2$ (where K is the coupling energy constant in the kT units) which is a correct result for $\beta\Gamma_{\text{eff}}$, obtained also from the Evans equation (Evans 1979, equation (A.28)) and extrapolation to $G = 0^+$ (Stecki and Dudowicz 1986a).

It is interesting to note that the main contribution to (3.8) comes from $\Delta z = 0$ and the successive $C^{\infty}_{\text{cond}2}(|\Delta z|)$ for $\Delta z \neq 0$ contribute less than 6% of the sum. Therefore the following approximation is proposed. It must be good at low temperatures.

$$\beta\Gamma(W=\infty) \simeq C^{\infty}_{\text{cond}2}(\Delta z = 0). \tag{3.9}$$

Figure 4(a) shows the existence of the limit of $C_{\text{cond}2}$ also demonstrating that the dependence on $(M+1)^{-2}$ is linear (unless the distance from the Gibbs dividing surface

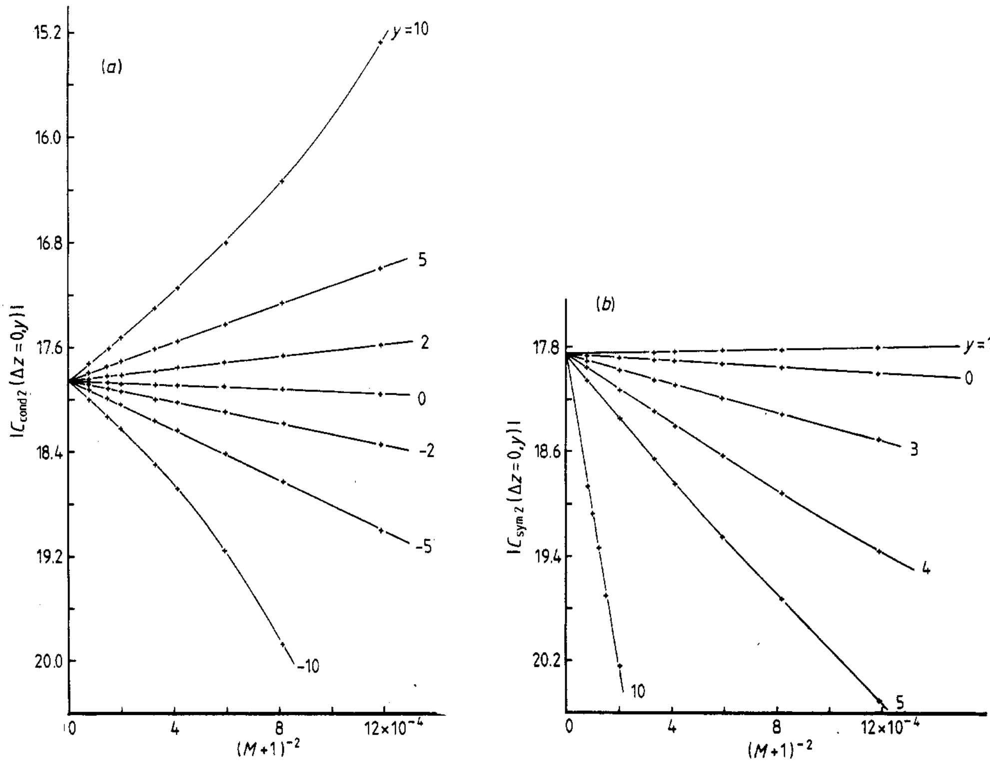

Figure 4. (a) The second moment $C_{\text{cond}2}$ ($\Delta z = 0$, y) of the conditional correlation function C_{cond} for a two-dimensional SOS ($M \times \infty$) system plotted against $(M+1)^{-2}$ at $T = 0.3T_c$, $G \equiv 0$, for various y, in the range $M = 28$–70. (b) The second moment $C_{\text{sym}2}$ of the symmetric correlation function C_{sym}; other details as for (a).

is large). The convergence of $C_{\text{cond2}}(z_1, z_2)$ to its asymptotic value $C^{\infty}_{\text{cond2}}(|\Delta z|)$ is achieved for any given z_1, z_2 irrespective of their values. The same conclusion refers to $C_{\text{sym2}}(z_1, z_2)$ and is shown in figure 4(*b*).

We discuss now the curious features of (3.6) or (3.7). In a shorthand notation (3.6) takes the form

$$\beta\Gamma(W) = A_1^{\text{cond}} + A_2^{\text{cond}}. \tag{3.10}$$

With the increasing system $M \to \infty$ (or $W \to \infty$)

$$A_1^{\text{cond}} \equiv -\tfrac{1}{2}\sum_{z_1} p(z_1) \sum_{z_2} C_{\text{cond2}}(z_1, z_2) \tag{3.11}$$

tends to zero as $(M+1)^{-2}$ (see figure 5(*a*)) and

$$A_2^{\text{cond}} \equiv \tfrac{1}{2}\sum_{z_1} p(z_1) \sum_{z_2} E_{\text{cond2}} \tag{3.12}$$

tends to $2s^2$ also as $(M+1)^{-2}$ (figure 5(*b*)).

Hence (3.6) produces (for $W \to \infty$) the correct result irrespectively of the order of the summation and taking the limit $W \to \infty$. However, $A_1^{\text{cond}} \to 0$ and $A_2^{\text{cond}} \to 2s^2$ if summations are carried out first and the limit $W \to \infty$ is taken next. When the order is reversed, A_1^{cond} produces $2s^2$ and A_2^{cond} vanishes.

The RHS of (3.7) gives zero or $2s^2$ depending on the order of summation and limit $W \to \infty$.

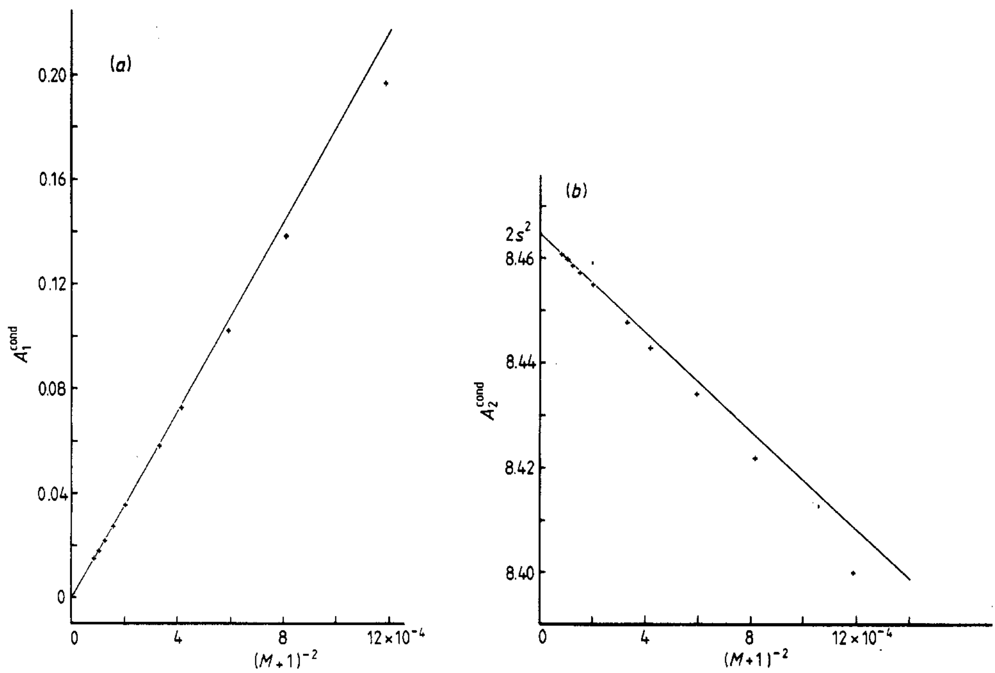

Figure 5. The contributions (*a*) A_1^{cond} (see equation (3.11)) and (*b*) A_2^{cond} (see equation (3.13)) to the interfacial tension $\beta\Gamma$ for two-dimensional SOS system ($M \times \infty$) as a function of $(M+1)^{-2}$ at $T = 0.3\,T_c$, $G \equiv 0$. M range 28–110.

Instead of substitution of (2.1) and (2.2) into the YTZ equation (3.1) we can use relations (2.11) and (2.12) between C and C_{sym}. After some algebra we find

$$\beta\Gamma(W) = -\tfrac{1}{2}\sum_{z_1} p(z_1)^{1/2} \sum_{z_2} p(z_2)^{1/2} C_{\mathrm{sym}2}(z_1, z_2)$$
$$+\sum_{z_1} p(z_1) \sum_{z_2} p(z_2)^{1/2}\nabla^-[p(z_2)^{1/2}]\nabla_1^- Q_2(z_1, z_2-1)$$
$$+\tfrac{1}{2}\sum_{z_1} p(z_1)^{1/2}\nabla^-[p(z_1)^{1/2}] \sum_{z_2} p(z_2)^{1/2}\nabla^-[p(z_2)^{1/2}] Q_2(z_1-1, z_2-1). \tag{3.13}$$

In a shorthand notation (3.13) becomes

$$\beta\Gamma(W) = A_1^{\mathrm{sym}} + A_2^{\mathrm{sym}} + A_3^{\mathrm{sym}}. \tag{3.14}$$

With $M \to \infty$ (and $W \to \infty$)

$$A_1^{\mathrm{sym}} \equiv -\tfrac{1}{2}\sum_{z_1} p(z_1)^{1/2} \sum_{z_2} p(z_2)^{1/2} C_{\mathrm{sym}2}(z_1, z_2) \tag{3.15}$$

tends to $s^2/2$ as $(M+1)^{-1}$ (figure 6(a)) and

$$A_2^{\mathrm{sym}} \equiv \sum_{z_1} p(z_1) \sum_{z_2} p(z_2)^{1/2}\nabla^-[p(z_2)^{1/2}]\nabla_1^- Q_2(z_1, z_2-1) \tag{3.16}$$

tends to $2s^2$ as $(M+1)^{-1}$ (figure 6(b)), whereas

$$A_3^{\mathrm{sym}} \equiv \tfrac{1}{2}\sum_{z_1} p(z_1)^{1/2}\nabla^-[p(z_1)^{1/2}] \sum_{z_2} p(z_2)^{1/2}\nabla^-[p(z_2)^{1/2}] Q_2(z_1-1, z_2-1) \tag{3.17}$$

tends to $-s^2/2$ also as $(M+1)^{-1}$ (figure 6(c)). All three quantities A_1^{sym}, A_2^{sym}, A_3^{sym} vary almost linearly with $(M+1)^{-1}$ and A_1^{sym} and A_3^{sym} cancel in the limit $W \to \infty$. So we find a new expression for the interfacial tension

$$\beta\Gamma(W) = \tfrac{1}{2}\sum_{z_1} p(z_1) \sum_{z_2} p(z_2)^{1/2}\nabla^-[p(z_2)^{1/2}]\nabla_1^- Q_2(z_1, z_2-1)$$
$$+\tfrac{1}{2}\sum_{z_1} p(z_2)^{1/2}\nabla^-[p(z_1)^{1/2}] \sum_{z_2} p(z_2)\nabla_2^- Q(z_1-1, z_2)$$

or

$$\beta\Gamma(W) = \sum_{z_1} p(z_1) \sum_{z_2} p(z_2)\nabla^-[p(z_2)^{1/2}]\nabla_1^- Q_2(z_1, z_2-1)$$
$$= \sum_{z_1} p(z_1)\nabla^-[p(z_1)^{1/2}] \sum_{z_2} p(z_2)\nabla_2^- Q_2(z_1-1, z_2)$$

which gives $\beta\Gamma_{\mathrm{eff}} = 2s^2$ for $W \to \infty$.

Figure 7 shows $\beta\Gamma$ against W^{-2}. The line (A) corresponds to $G=0$ and a series of M, the line (B) corresponds to a series of G vanishing to zero; both are computed from the YTZ equations (3.1) or (3.6) which are equivalent. The line (C) was computed earlier from the Evans equation (Evans 1979, equation (A.28)) (Stecki and Dudowicz 1986a). However, no universal common curve is observed; the asymptotic limit $\beta\Gamma(W=\infty)$ is the same $(2s^2)$ for all three cases as well as the linear dependence of $\beta\Gamma(W)$ on W^{-2}.

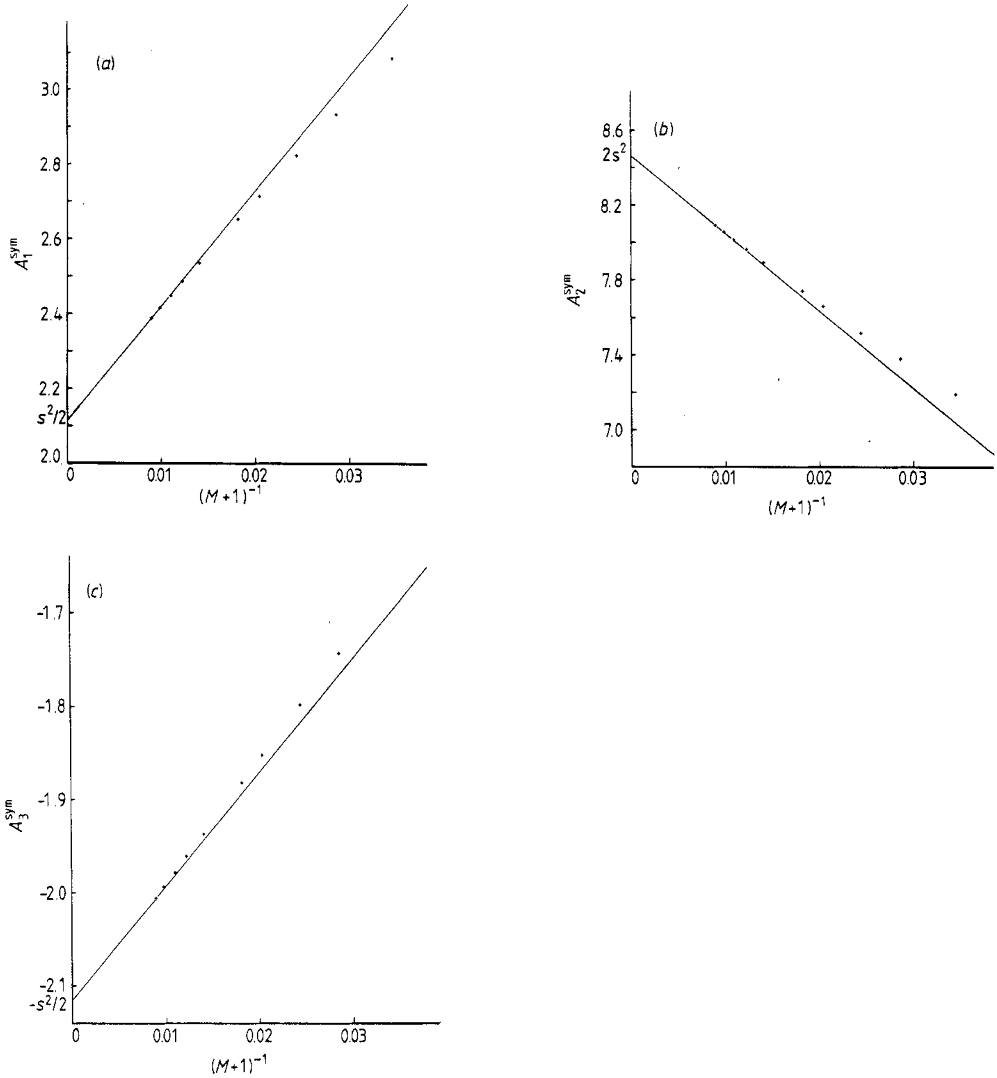

Figure 6. The contributions (*a*) A_1^{sym} (see equation (3.15)), (*b*) A_2^{sym} (see equation (3.16)) and (*c*) A_3^{sym} (see equation (3.17)) to the interfacial tension $\beta\Gamma$ for a two-dimensional $(M\times\infty)$ SOS system as a function of $(M+1)^{-1}$ at $T=0.3T_c$, $G\equiv 0$, for the range $M=$ 28–110.

4. Discussion

In the absence of an external field, the infinite sizes of the system correspond to an infinite interface width W. Then the second moment C_2, of the direct correlation function C, diverges. The original YTZ formula for interfacial tension ((3.1), has been modified so that the resulting equation (3.8) is valid in the limit $W\to\infty$ (Ciach *et al* 1987) directly. It contains one summation (integration) over the relative distance Δz. Since we find that the main contribution ($\sim$95%) to $\beta\Gamma(\infty)=2s^2$ comes from $C^{\infty}_{\mathrm{cond2}}(\Delta z=0)$, the following approximation seems reliable at low temperatures

$$2\beta\Gamma^{\infty}=-C^{\infty}_{\mathrm{cond2}}(\Delta z=0).$$

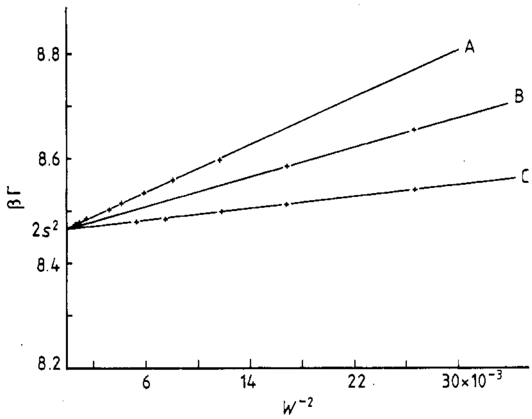

Figure 7. The interfacial tension $\beta\Gamma$ at $T = 0.3\,T_c$ for a two-dimensional SOS system ($M \times \infty$) plotted against the interface width W^{-2}; the line (A) corresponds to $G \equiv 0$, $W = (M+1)/\pi$ and the YTZ equation (3.1); the line (B) corresponds to a series of G vanishing to zero, $W = [G^{-1/4}(2s)^{-1/2}]$ and the YTZ equation (3.1); and the line (C) was computed from the Evans equation (Evans 1979, equation (A.28)).

The second moment E_{cond2} of the 'correction' term E_{cond} (2.2), tends to zero and C_{cond2} tends to $C^{\infty}_{\text{cond2}}$. We have studied here the limiting behaviour of these quantities and we find that

$$\lim_{W\to\infty} \int_{-\infty}^{\infty} \mathrm{d}z f(z, W) \neq \int_{-\infty}^{\infty} \mathrm{d}z \lim_{W\to\infty} f(z, W).$$

Therefore, as described in § 3, the contributions to $\beta\Gamma(W=\infty)$ depend on the order of summation (integration) and taking the limit $W = \infty$. The interfacial tension $\beta\Gamma(W)$ for $G \equiv 0$ is also compared with $\beta\Gamma(W)$ calculated for a series of vanishing G by using the original YTZ formula (3.1) or by using the Evans equation (Evans 1979, equation (A.28)). The limiting value $\beta\Gamma(W=\infty)$ is common for these three cases. And indeed in the limit $W = \infty$ the YTZ formula and the Evans formula (A.28) are equivalent.

For $W < \infty$, in these three cases no universal curve $\beta\Gamma(W)$ is found. Figure 7 shows three (linear) plots of $\beta\Gamma(W)$ against W^{-2}, with an extrapolated common value $\beta\Gamma(\infty)$ but with three different slopes. We also note that the plot is linear to a much better approximation for $G > 0$.

Acknowledgment

I wish to express my gratitude to Professor Jan Stecki for a critical reading of the manuscript, many helpful discussions during this work and his constant advice and interest.

Appendix

For a finite SOS system ($M \times \infty$), the Fourier transform of the height-height correlation function $P(h_1, h_2)$ (Stecki 1984) is computed by the method described earlier, with the aid of eigenvectors x_i and eigenvalues λ_i of a column-column transfer matrix $\mathbf{T}$ (see, for example, Stecki and Dudowicz 1986b):

$$\tilde{P}(h_1, h_2; k_\perp) = P(h_1, h_2; \Delta x = 0) + 2 \sum_{J \geq 2} x_n^{(1)} x_m^{(1)} x_n^{(J)} x_m^{(J)} \frac{R_J(\cos k_\perp - R_J)}{1 - 2R_J \cos k_\perp + R_J^2} \quad \text{(A1)}$$

where $R_i \equiv \lambda_i / \lambda_1$, $n = h_1 + 1$ and $m = h_2 + 1$. The inversion of matrix $\tilde{\mathbf{P}}(k_\perp)$ produces the matrix $\tilde{\mathbf{Q}}(k_\perp)$

$$\tilde{\mathbf{Q}}(k_\perp) = \tilde{\mathbf{P}}(k_\perp)^{-1} \quad \text{(A2)}$$

and the Orstein-Zernike correlation function C can be obtained from the formula (Stecki 1984):

$$\tilde{C}(z_1 = h_1, z_2 = h_2; k_\perp) = \nabla_1^- \nabla_2^- \tilde{Q}(z_1 = h_1, z_2 = h_2; k_\perp). \quad \text{(A3)}$$

The inversion of $\tilde{\mathbf{P}}(k_\perp)$ as well as the diagonalisation of matrix $\mathbf{T}$ was done numerically on a CDC 6400 in double precision. Only then were the values reliable.

It is remarkable that calculation of $\tilde{C}(k_\perp)$ via $\tilde{P}(k_\perp)$ (see (A1)-(A3)) is associated with the almost tenfold decrease of computer time, compared with the standard method described elsewhere (Stecki and Dudowicz 1986a, b) via $\tilde{H}(k_\perp)$ and then inverting $\tilde{H}(k_\perp)$ into $\tilde{C}(k_\perp)$.

Carrying out this procedure (A1)-(A3) first for $k_\perp = 0$ and then for $k = \pi/2$, we find the second moment of C, $C_2 = 2C(\Delta x = 1)$ from the relation (2.6).

Equations (A2) and (A3) are also valid in their application to C_{cond} and C_{sym}

$$\tilde{C}_{\text{cond}}(z_1, z_2; k_\perp) = \nabla_1^- \nabla_2^- \tilde{Q}_{\text{cond}}(z_1, z_2; k_\perp) \quad \text{(A4)}$$

$$\tilde{C}_{\text{sym}}(z_1, z_2; k_\perp) = \nabla_1^- \nabla_2^- \tilde{Q}_{\text{sym}}(z_1, z_2; k_\perp) \quad \text{(A5)}$$

$$\tilde{\mathbf{Q}}_{\text{cond}}(k_\perp) = \tilde{\mathbf{P}}_{\text{cond}}(k_\perp)^{-1} \quad \text{(A6)}$$

$$\mathbf{Q}_{\text{sym}}(k_\perp) = \tilde{\mathbf{P}}_{\text{sym}}(k_\perp)^{-1} \quad \text{(A7)}$$

where the correlation function $P_{\text{cond}}(z_1, z_2)$ and $P_{\text{sym}}(z_1, z_2)$, invented by Ciach (1986), are defined as

$$P_{\text{cond}}(z_1, z_2; \Delta x) = P(z_1, z_2; \Delta x)/p(z_1) \quad \text{(A8)}$$

$$P_{\text{sym}}(z_1, z_2; \Delta x) = P(z_1, z_2; \Delta x)/[p(z_1)p(z_2)]^{1/2}. \quad \text{(A9)}$$

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