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Correlation functions in the two-dimensional Gaussian-column model of the interface in a weak external field

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Abstract. Calculations of the correlation functions C and $C_{\rm cond}$ for the two-dimensional Gaussian-column model of the interface in a weak gravitational field, $G \to 0^+$, indicate the universality of the parametrisation of the direct correlation function C, found for the SOS model by Stecki, Ciach and Dudowicz. The representations of the conditional correlation function $C_{\rm cond}$ are slightly different in these two models.

1. Introduction

The structure of the interface as described by the correlation functions, interfacial tension and susceptibilities has been studied recently (Stecki and Dudowicz 1986a, b, Stecki *et al* 1986, Ciach *et al* 1987, Dudowicz 1988, Hemmer and Lund 1988). These studies concerned the interface between two coexisting fluid phases represented by the two-dimensional ($d=2$) ($M \times \infty$) solid-on-solid model. The interface is localised by the presence of the external field G and/or the finite size of the system; otherwise fluctuations are unbounded. It is known that any external potential, however weak, pins the interface even in two dimensions (van Leeuwen and Hilhorst 1981). Interesting analytical studies of solid-on-solid models and wetting in two dimensions in external fields were carried out by Privman and Svrakic (1988).

In a recent extension of these results to three dimensions ($d=3$), Ciach (1987) found a non-analyticity of the Fourier transform of C in the transverse direction, in contradiction with the usual assumptions.

We have extracted some 'intrinsic' quantities, i.e. quantities that exist in the limit of infinite interface width, $W \to \infty$. The latter can be obtained either in the limit of weak external field, $G \to 0^+$, or for system sizes increasing indefinitely. In other words, there are some quantities which diverge as $W \to \infty$, some which vanish, some which are ill defined and some which obtain well defined limiting values. The latter are intrinsic properties, examples of which are the interfacial tension and the correlation lengths of suitably redefined two-point functions. Neither the density profile nor the susceptibilities are intrinsic properties.

For the Orstein-Zernike direct correlation function C in the SOS interface in the limit of $G \to 0^+$, the following representation was found (Stecki *et al* 1986):

$$\tilde{C}(k_\perp; \Delta z, Z) = \sqrt{\pi}\, W \exp[(1+B(\Delta z)G^{1/2})(Z/W)^2] M(|\Delta z|; k_\perp) \qquad (1.1)$$

where $\tilde{C}(k_\perp; \Delta z, Z)$ is the Fourier transform of $C(\Delta x; \Delta z, Z)$ and $k_\perp$ is the Fourier variable in the transverse direction x. The coefficient $B(\Delta z)$ and the matrix $M(\Delta z; k_\perp)$

depend on the relative distance $\Delta z = z_2 - z_1$ only, the other distance variable Z is defined as $Z = (z_1 + z_2 - 2z_0)/2$ where z_0 corresponds to the middle of the system. The interface width W is

$$W = G^{-1/4}(2\sinh\beta J)^{-1/2} \tag{1.2}$$

where J is the coupling energy constant and $\beta = 1/kT$.

Recent asymptotic calculations by Hemmer and Lund (1988) for weak gravitational fields confirmed the validity of parametrisation (1.1), i.e. fast variation with Δz and slow variation with Z/W.

It was also found that in the limit of $G \to 0^+$ the matrix $M(\Delta z; k_\perp)$ takes the form

$$M(\Delta z; k_\perp) = t + A\exp(-|\Delta z|/\xi_\parallel) \tag{1.3}$$

where t is a tridiagonal matrix, A is a temperature-dependent coefficient and $\xi_\parallel$ is the longitudinal (in the z direction) correlation length. In the limit of $G \to 0$ ($W \to \infty$), M is identical with the conditional correlation function C_{cond}, introduced by Ciach (1986); she also found expression (1.3) with

$$\xi_\parallel^{-1} = -\ln(D - \sqrt{D^2 - 1}) \qquad D = 2\cosh 2\beta J - 1. \tag{1.4}$$

In the present paper we check the universality of (1.1)-(1.3) by studying a slightly different model of the interface, i.e. the Gaussian-column model which produces, at a given temperature, a smoother and less fluctuating interface. Both models take into account only nearest-neighbour interactions, and are represented by Hamiltonians belonging to the same class $H = \Sigma_i\, 2\beta J|h_i - h_{i+1}|^\alpha$, with exponent $\alpha = 2$ for the Gaussian model and $\alpha = 1$ for the SOS model. For the Gaussian model smaller external fields are sufficient to ensure an accurate extrapolation of computed functions to their limiting values for $G \to 0^+$.

2. Parametrisation of the direct Orstein–Zernike correlation function

The Gaussian model of the interface was introduced by Chui and Weeks (1976) and was then applied to studies of interfacial phenomena by many authors (see, for example, Chui and Weeks (1978), Weeks (1977) and Bedaux *et al* (1985)).

The system is a two-dimensional array ($M \times \infty$) of columns of heights $\{h_i\}$, $0 \leqslant h \leqslant M$, with periodic boundary conditions in the x direction, $-\infty < i < \infty$. The column-column interaction energy is

$$E = 2J\beta \sum_i |h_i - h_{i+1}|^2 \qquad J > 0. \tag{2.1}$$

The external potential $V^{\text{ext}}(h)$ pinning the interface

$$V^{\text{ext}}(h) = G|h - h_0|^2 \qquad G > 0 \tag{2.2}$$

represents the gravitational potential (van Leeuwen and Hilhorst 1981) and h_0 corresponds to the middle of the system. So the energy H of the interface, up to an arbitrary constant, is given by

$$H = E(\{h_i\}) + \sum_i V^{\text{ext}}(h_i). \tag{2.3}$$

The method of computation we shall use is the transfer matrix technique described elsewhere (Stecki and Dudowicz 1986b).

We begin with the determination of the interface width W. Usually, W and the probability, $p(h)$, that a single column has height h (or $p(z)$ in variables z) are related by

$$p(z)=\frac{\exp[-(z-z_0)^2/W^2]}{\sqrt{\pi}W} \tag{2.4}$$

and $p(z)$, in turn, is usually related to the density profile by

$$p(z)=-\nabla\rho(z)=\rho(z)-\rho(z-1). \tag{2.5}$$

Equations (2.4) and (2.5) are used for determining W for a given size M (G is assumed to take a value which does not change the eigenvalues λ_i and eigenvectors $\boldsymbol{x}_i$ of the $(M+1)\times(M+1)$ transfer matrix $\mathbf{T}$, in terms of which all the quantities under study can be expressed (Stecki and Dudowicz 1986b)). Figure 1 shows that

$$W=G^{-1/4}\times\text{constant}. \tag{2.6}$$

By employing the computed values of W, one obtains the universal density profile, $\rho(y=|z-z_0|/W)$, common for all systems of sizes $(M\times\infty)$ (see figure 2). This confirms the universality of the asymptotic exponent, $-1/4$, of G.

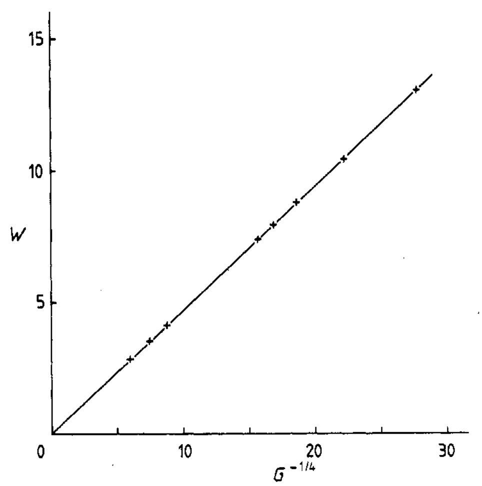

Figure 1. The linear variations of the interface width W calculated from probability $p(z_0)$ (see equations (2.4) and (2.5)) with the external field $G^{-1/4}$ for a two-dimensional $(M\times\infty)$ Gaussian-column model at $T=0.3T_c$ in the range of $M=29$–109. T_c is related to the Ising model.

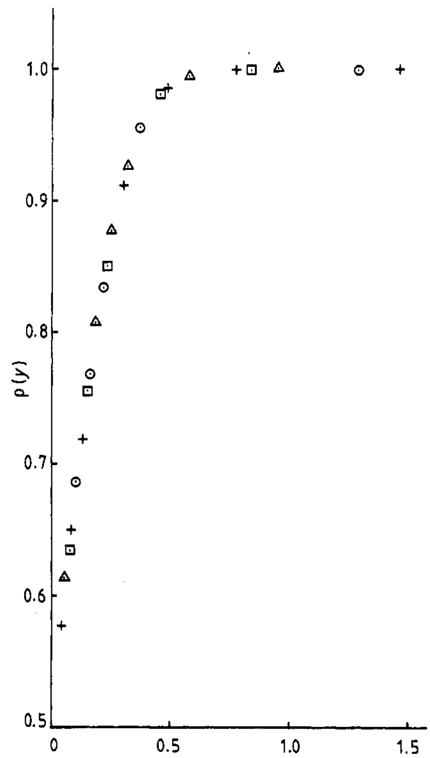

Figure 2. The density $\rho(y)$ against $y=|z-z_0|/W$ at $T=0.3T_c$. Data points □ ($G=1.666\,66\times10^{-4}$), △ ($G=8.333\,33\times10^{-5}$), ⊙ ($G=4.166\,66\times10^{-5}$) and + ($G=1.666\,66\times10^{-5}$) fall on a common curve.

The validity of representation (1.1) extended to the Gaussian model is shown in a very convincing way by plotting

$$A_0 = (W/Z)^2 \ln\left(\frac{\tilde{C}(k_\perp = 0; \Delta z, Z)}{\tilde{C}(k_\perp = 0; \Delta z, Z = 0)}\right) \tag{2.7}$$

against $G^{1/2}$ (figure 3). All curves corresponding to a given value of $|\Delta z|$ meet at $G = 0$ at a common value $A_0 = 1$. If we try to extend the exponential term in expression (1.1) to a more general form

$$\exp[A_0(Z/W)^2 + A_2(Z/W)^4 + A_4(Z/W)^6] \tag{2.8}$$

we find that $A_2 = A_4 = 0$ in the limit $G \to 0^+$, as was obtained for the SOS interface by Stecki and Dudowicz (1986a). The longitudinal correlation length $\xi_\parallel$ may also be computed from the relation

$$\xi_\parallel^{-1} = -\tfrac{1}{2} \ln\left(\frac{\tilde{C}(k_\perp = 0; |\Delta z| + 2, Z)}{\tilde{C}(k_\perp = 0; |\Delta z|, Z)}\right) \qquad |\Delta z| \geqslant 2 \tag{2.9}$$

and is shown for a few pairs Δz, Z as a function of $G^{1/2}$ in figure 4. An analytical expression for $\xi_\parallel$ (like equation (1.4)) for the Gaussian model has not been derived. The longitudinal correlation length $\xi_\parallel$ is common to the direct correlation function C

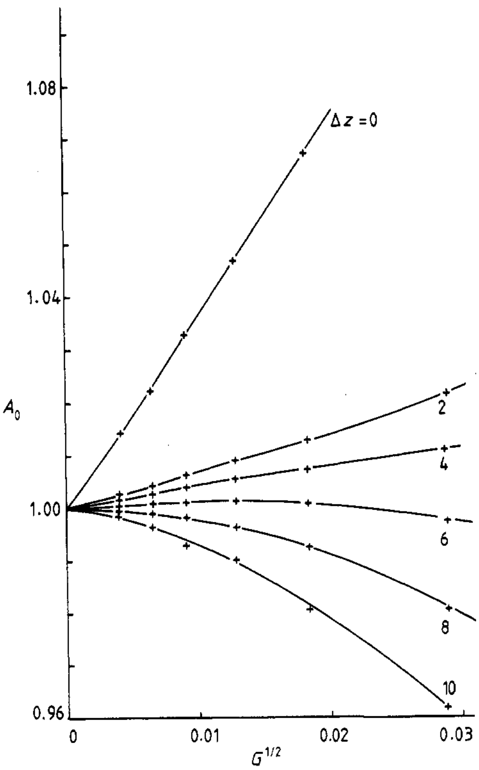

Figure 3. The coefficient A_0 computed from (2.7) plotted against $G^{1/2}$ at $T = 0.3T_c$. Curves are labelled with the value of $|\Delta z| = |z_2 - z_1|$.

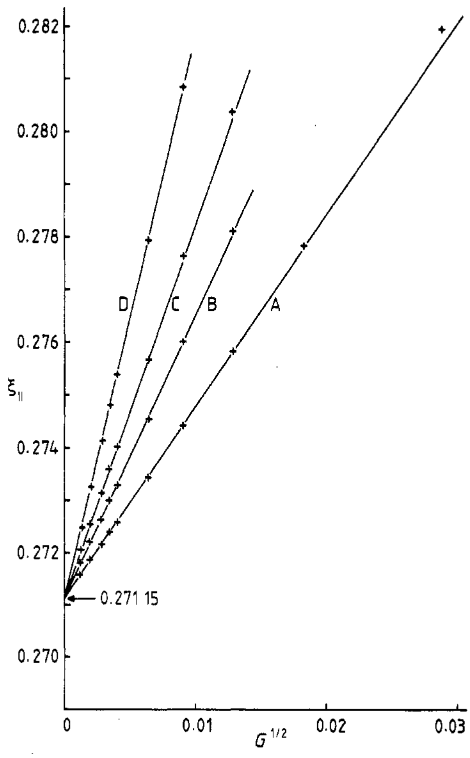

Figure 4. The longitudinal correlation length $\xi_\parallel$ computed from (2.9) as a function of $G^{1/2}$ at $T = 0.3T_c$. Lines A, C and D correspond to $Z = 0$ and $\Delta z = 2, 4$ and 6 respectively, line B corresponds to $Z = \frac{1}{2}$ and $\Delta z = 3$. The intercept $\xi_\parallel^\infty = 0.271\,15$.

and the conditional correlation function C_{cond}. The conditional correlation function C_{cond}, introduced for the first time by Ciach (1986) is of the order of unity, whereas C is of order W. For $W \to \infty$ $(G \to 0^+)$ C_{cond} takes its limiting value C^{∞}_{cond} which is a function of the relative distance $|\Delta z|$ only. Figure 5 shows the convergence of $\tilde{C}_{\text{cond}}(k_\perp = 0, \Delta z, Z)$ for $\Delta z = 0$ and various Z to one asymptotic value $\tilde{C}^{\infty}_{\text{cond}}(k_\perp = 0, \Delta z = 0)$. When $\Delta z \neq 0$ we obtain for each Z two curves $\tilde{C}_{\text{cond}}(k_\perp = 0; \Delta z)$ against $G^{1/2}$—one corresponding to positive Δz, the other to negative Δz, since C_{cond} is not symmetrical with respect to the interchange of z_1 and z_2. These two curves, however, converge in the asymptotic limit $G \to 0^+$ to the limiting value $\tilde{C}^{\infty}_{\text{cond}}(k_\perp = 0; |\Delta z|)$ (see figure 6).

We find that $\tilde{C}_{\text{cond}}$ in the Gaussian model can be expressed as

$$\tilde{C}_{\text{cond}}(k_\perp = 0; \Delta z, Z) = D_t + (-1)^{|\Delta z|} E \exp(-|\Delta z|/\xi_\parallel) \tag{2.10}$$

where D_t is a tridiagonal matrix with non-zero elements for $\Delta z = 0$, ± 1. E is a temperature-dependent coefficient and $\xi_\parallel$ is the longitudinal correlation length, which can be computed from the expression, similar to (2.9),

$$\xi_\parallel^{-1} = -\tfrac{1}{2} \ln \left(\frac{\tilde{C}_{\text{cond}}(k_\perp = 0, \Delta z \pm 2, Z)}{\tilde{C}_{\text{cond}}(k_\perp = 0, \Delta z, Z)} \right) \qquad |\Delta z| \geq 2 \tag{2.11}$$

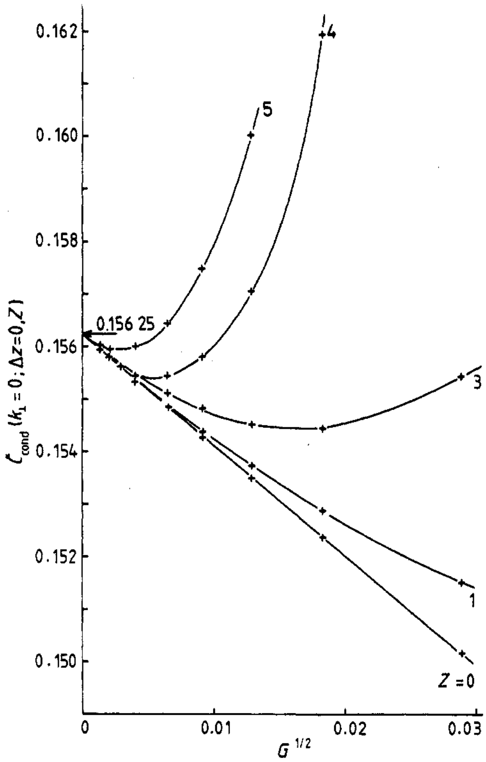

Figure 5. The Fourier transform of the conditional correlation function, $\tilde{C}_{\text{cond}}(k_\perp = 0; \Delta z = 0, Z)$ plotted against $G^{1/2}$ at $T = 0.3T_c$. Curves are labelled with the value of $Z \equiv (z_1 + z_2 - 2z_0)/2$. The intercept $\tilde{C}^{\infty}_{\text{cond}}(k_\perp = 0; \Delta z = 0) = 0.156\,25$.

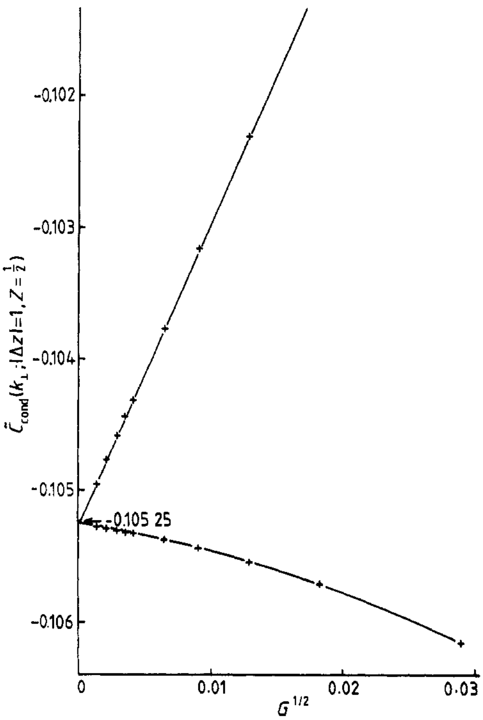

Figure 6. The Fourier transform of the conditional correlation function $\tilde{C}_{\text{cond}}(k_\perp = 0, |\Delta z| = 1, Z = \frac{1}{2})$ plotted against $G^{1/2}$ at $T = 0.3T_c$. The upper curve corresponds to $\Delta z = 1$ and the lower one to $\Delta z = -1$. These two curves converge to a common value of $-0.105\,25$ at $G^{1/2} = 0$.

where $\Delta z+2$ corresponds to positive Δz and $\Delta z-2$ corresponds to negative Δz. Extrapolation of $\xi_\parallel$ to $G\to 0^+$ gives the same value for all pairs Δz, Z, which is identical with $\xi_\parallel^\infty$ extracted from the direct correlation function C. According to (2.10) the coefficient E can be found from

$$E=\frac{(\tilde{C}_{\text{cond}}(k_\perp=0,\Delta z=2,Z))^2}{C_{\text{cond}}(k_\perp=0,\Delta z=4,Z)}. \tag{2.12}$$

The extrapolated (to $G\to 0^+$) value $E^\infty=44.422$ (see figure 7) is in excellent agreement with

$$E^\infty=\frac{\tilde{C}^\infty_{\text{cond}}(k_\perp=0,|\Delta z|)}{\exp(-|\Delta z|/\xi_\parallel^\infty)} \qquad |\Delta z|\geqslant 2. \tag{2.13}$$

Determination of E^∞ makes it possible to find the elements of the tridiagonal matrix D_t. From (2.10) we have

$$D_t^\infty(\Delta z=0)=\tilde{C}^\infty_{\text{cond}}(k_\perp=0,\Delta z=0)-E^\infty \tag{2.14}$$

$$D_t^\infty(|\Delta z|=1)=\tilde{C}^\infty_{\text{cond}}(k_\perp=0,|\Delta z|=1)+E^\infty\exp(-1/\xi_\parallel). \tag{2.15}$$

The matrix $M(\Delta z)$ in representation (1.1) is simply $\tilde{C}^\infty_{\text{cond}}(\Delta z)$ for $W\to\infty$. Extrapolation to $G\to 0^+$ of the elements of $M(\Delta z, k_\perp=0)$ computed from the simplified form of (1.1) (with $B=0$)

$$M(\Delta z,k_\perp=0)=\frac{\tilde{C}(k_\perp=0,\Delta z,Z)}{\sqrt{\pi}W}\exp[-(Z/W)^2] \tag{2.16}$$

gives exactly $\tilde{C}^\infty_{\text{cond}}(k_\perp=0,|\Delta z|)$.

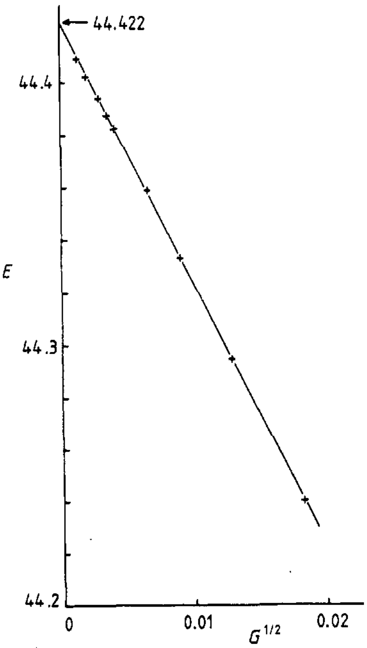

Figure 7. The coefficient E defined by (2.10) and computed from (2.12) plotted against $G^{1/2}$ for $T=0.3T_c$. The intercept $E^\infty=44.422$.

Table 1. Comparison of the values found for various quantities in the Gaussian and SOS models. Note that $T=0.3T_c$ (Ising), i.e. $\beta J=0.4407/0.3$.

	Gaussian model	SOS model
$WG^{1/4}=\text{constant}$	0.467 85	
$WG^{1/4}=(2\sinh\beta J)^{-1/2}$		0.492 99
$\xi_{\parallel}^{\infty}$	0.271 15	0.279 42
E^{∞}	44.422	32.020
$D_t^{\infty}(\Delta z=0)$	−44.266	−31.859
$D_t^{\infty}(\lvert\Delta z\rvert=1)$	1.006 3	−1
$\tilde{C}_{\text{cond}}^{\infty}(k_\perp=0;\Delta z=0)$	0.156 25	0.161 39
$\tilde{C}_{\text{cond}}^{\infty}(k_\perp=0;\lvert\Delta z\rvert=1)$	−0.105 25	−0.106 35
$\tilde{C}_{\text{cond}}^{\infty}(k_\perp=0;\lvert\Delta z\rvert=2)$	0.027 812	0.024 941
$\tilde{C}_{\text{cond}}^{\infty}(k_\perp=0;\lvert\Delta z\rvert=3)$	$-0.684\,0\times10^{-3}$	$0.695\,0\times10^{-3}$
$\tilde{C}_{\text{cond}}^{\infty}(k_\perp=0;\lvert\Delta z\rvert=4)$	$0.174\,13\times10^{-4}$	$0.194\,27\times10^{-4}$

Table 1 contains $\tilde{C}_{\text{cond}}^{\infty}(k_\perp=0;|\Delta z|)$ for a few small values of $|\Delta z|$ and other quantities (equations (2.9)-(2.15)) extrapolated to the asymptotic limit $W\to\infty$. The corresponding values for the SOS system are also presented for comparison. We also expect (2.10) to be valid for $k_\perp\neq0$.

3. Discussion and comparison of the Gaussian-column model with the SOS model

As we show in § 2, the representation of the direct correlation function C (1.1) obtained earlier for the SOS model of the interface by Stecki *et al* (1986) exhibits features of universality. The asymptotic exponent scaling the interface width W with the external field G is also universal and equal to $-\frac{1}{4}$. The longitudinal correlation length $\xi_{\parallel}$ and other coefficients of relation (1.1) change linearly for two models with $G^{1/2}$ (see figures 4 and 7). The known equation (Stecki 1984) found for the SOS model

$$\tilde{C}(k_\perp;z_1,z_2)=C(\Delta x=0;z_1,z_2)+2C(\Delta x=1;z_1,z_2)\cos k_\perp$$

with $C(\Delta x)=0$ for $|\Delta x|\geq2$, is also universal.

However, the representations of $\tilde{C}_{\text{cond}}(k_\perp)$ in these two models are a little different (see equations (1.3) and (2.10)). They differ by a factor $(-1)^{|\Delta z|}$, which gives rise to an oscillating character of $\tilde{C}_{\text{cond}}(k_\perp)$ in the Gaussian model (positive for even values of Δz, negative for odd Δz) compared with a smooth behaviour of $\tilde{C}_{\text{cond}}$ in the SOS model (for all Δz, except $|\Delta z|=1$, $\tilde{C}_{\text{cond}}>0$). The direct correlation function $\tilde{C}$ for the Gaussian model also exhibits an oscillating character, but in spite of this the parametrisation (1.1) is valid since the oscillating behaviour is included in $\tilde{C}_{\text{cond}}(k_\perp)$ (or $M(k_\perp,\Delta z)$). The fact that there is reasonable agreement, between the two models for the values of $\xi_{\parallel}$ and other quantities summarised in table 1 is a consequence of the low temperature.

We have also compared the effective interfacial tension which is a measure of surface stiffness and is an intrinsic property of the interface. For the SOS model we found linear variation with $\sqrt{G}$ (Stecki and Dudowicz 1986a):

$$\beta\Gamma^{\text{eff}}(G)=\beta\Gamma^{\text{eff}}(0)+\alpha_1\sqrt{G}\qquad\beta\Gamma^{\text{eff}}(0)=2\sinh^2(\beta J)$$

and this is also found to be valid for the Gaussian model. We find

$$\beta\Gamma^{\text{eff}}(0)_{\text{Gauss}}>\beta\Gamma^{\text{eff}}(0)_{\text{SOS}}$$

and

$$\alpha_1^{(\mathrm{Gauss})} < \alpha_1^{(\mathrm{SOS})}.$$

These inequalities are consistent with the greater stiffness of the Gaussian interface.

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