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Gradient expansion of the distribution function in the two-dimensional SOS model†

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Abstract. The distribution function $\langle\sigma\sigma\rangle$ in the inhomogeneous interface zone modelled by a two-dimensional SOS (solid-on-solid) system is successfully represented as polynomials in local density and the lattice analogues of its gradients and higher derivatives.

1. Introduction

The structure of the inhomogeneous interface between two coexisting phases is described in terms of the density profile and the two-point density-density distribution function. Simple lattice models for which the exact numerical computations can be carried out, are very useful even in two dimensions (Weeks 1977, van Leeuwen andHilhorst 1981, Stecki 1984, Dudowicz 1984, Stecki and Dudowicz 1984a, b, 1985a, b, Abraham 1984‡). These computations show that the distribution function in the two-dimensional system strongly depends on the external potential which also determines the shape of the density profile. But the density functional theory tells us that nevertheless it should be possible to eliminate the external field in favour of the density function, i.e. density profile $\rho(z)$.

In the present paper, it is shown how the SOS distribution function $\langle\sigma\sigma\rangle$ in the transverse direction depends on ρ, and its finite differences $\Delta\rho$ and $\Delta\Delta\rho$. The SOS model is recalled in § 2 together with the expressions for the density profile and pair distribution function needed in the context of the transfer matrix used for all computations. The geometry and the external field of the simulated system are established in § 3. In § 4 the representation of the transverse distribution function $\langle\sigma\sigma\rangle$ for $\Delta x = 1$, as polynomial in local density and its gradients is examined. A summary and discussion are given in § 5.

2. SOS model

The solid-on-solid (SOS) model is a low-temperature approximation to the interface which considers arrays of columns of occupied sites (Weeks 1977). Thus 'overhanging' configurations are eliminated and neither clusters of particles in the 'gas' ($\rho_G = 0$) nor

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‡ See also the references therein.

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holes in the 'liquid' phase ($\rho_L = 1$) are present. This picture is accurate for interfaces at low temperatures. The partition function is

$$Z = \sum_{\{h_i\}} \exp[-\beta E(\{h_i\})] \prod_i \exp[-\beta V_i^{\text{ext}}(h_i)], \tag{2.1}$$

where h_i denotes the height of column i and $\{h_i\} = \{h_1, h_2, \ldots\}$. Here E is the interaction energy of two neighbouring columns

$$E = 2J \sum_i |h_i - h_{i+1}| \qquad J > 0 \tag{2.2}$$

and the energy zero corresponds to a perfectly flat interface. V_i^{ext} is an external potential. The role of the external potential is to localise the interface and to limit its width which is divergent for $V_i^{\text{ext}} = 0$. It is known that infinitesimal external potential is sufficient to pin the interface even in two dimensions (van Leeuwen and Hilhorst 1981). Equations (2.1) and (2.2) show that instead of occupation numbers $\nu(x, z) = 0, 1$ of the lattice gas, the column heights $h(x)$, $0 \leqslant h(x) < \infty$ are used as microscopic variables (Chui and Weeks 1981, Jasnow *et al* 1982).

For the numerical computation of the distribution function we use the column-column transfer matrix. It is defined as

$$T_{mn} = T_{nm} = \exp[-\beta V^{\text{ext}}(m)/2 - \beta V^{\text{ext}}(n)/2 - 2\beta J|m-n|] \tag{2.3}$$

where $m = h+1$, $n = h'+1$ label the states of a single column, $0 \leqslant h \leqslant M$, M is taken large but fixed. The $(M+1)\times(M+1)$ symmetrical transfer matrix (2.3) has been diagonalised numerically with the aid of EISPACK routines producing eigenvalues λ_I and eigenvectors $\boldsymbol{x}^{(I)}$. Then by using the eigenvalue expansion

$$T_{mn} = \sum_{I \geqslant 1} x^{(I)}(m) \lambda_I x^{(I)}(n) \tag{2.4}$$

one can express various quantities (such as density profile, two-point distribution function) in terms of λ_I and $\boldsymbol{x}^{(I)}$. We use periodic boundary conditions in direction x throughout. The density profile is

$$\rho(z) = \sum_{h > z} [x^{(1)}(h)]^2. \tag{2.5}$$

Here, $x^{(1)}$ belongs to the largest eigenvalue, λ_1. For the two-particle distribution function, we obtain

$$\rho_2(z_1, z_2; \Delta x) = \sum_{h > z_1} \sum_{h > z_2} \sum_{I \geqslant 1} x^{(1)}(h) x^{(1)}(h') x^{(I)}(h) x^{(I)}(h') r_I^{\Delta x}, \tag{2.6}$$

where $r_I = \lambda_I / \lambda_1 < 1$, $\Delta x = |x_2 - x_1|$. In working equations the term $I = 1$ was separated out. These relations are valid in the limit $L \to \infty$ (L is the size in direction x in which the system is translationally invariant with periodic boundary conditions). One also defines the distribution function g through

$$\rho_2(z_1, z_2; \Delta x) = g(z_1, z_2; \Delta x) \rho(z_1) \rho(z_2). \tag{2.7}$$

3. Description of the system

The system studied is a sos $M \times \infty$ strip of quadratic lattice, $1 \leqslant z \leqslant M$, $1 \leqslant x < \infty$, with periodic boundary conditions in the x direction. The external field $V_i^{\text{ext}}(h)$ needed to

stabilise the interface may be taken as

$$V_x^{\text{ext}}(h) = \sum_{z=1}^{h} u^{\text{ext}}(x, z) \tag{3.1}$$

and

$$u^{\text{ext}}(x, z) = \begin{cases} -u_0 & z < z_0 \qquad u_0 > 0 \\ 0 & z = z_0 \\ u_0 & z > z_0. \end{cases} \tag{3.2}$$

u^{ext} is zero for the central layer and favours a particle for $z < z_0$ and a hole for $z > z_0$; it does not depend on the coordinate x. Hence, if $h_0 = z_0$ (or $h_0 = z_0 - \frac{1}{2}$) and separating a constant V_{00},

$$V_x^{\text{ext}}(h) = V_{00} - u_0|h - h_0|. \tag{3.3}$$

This is a particular case $\alpha = 1$ of $V^{\text{ext}} = g|h - h_0|^{\alpha}$; $\alpha = 2$ would correspond to the gravitational potential (van Leeuwen and Hilhorst 1981).

The system exhibits the particle-hole symmetry which leads to an antisymmetric density profile and symmetric (spin-spin) distribution function

$$\rho(z_0 + n) + \rho(z_0 - n) = 1 \qquad \rho(z_0) = 0.5, \tag{3.4}$$

$$\langle \sigma(z_0 + n_1, x)\sigma(z_0 + n_2, x \pm \Delta x)\rangle = \langle \sigma(z_0 - n_1, x)\sigma(z_0 - n_2, x \pm \Delta x)\rangle, \tag{3.5}$$

where $z_0 = z_{\text{mid}} = \frac{1}{2}M$ (M even) or $\frac{1}{2}(M+1)$ (M odd), n_1 and n_2 are integer numbers. The relation between $\langle\sigma\sigma\rangle$ and ρ_2 (see (2.6)) is the following:

$$\langle \sigma\sigma \rangle = 4\rho_2(z_1, z_2; \Delta x) - 2\rho(z_1) - 2\rho(z_2) + 1. \tag{3.6}$$

The distribution functions $\rho_2(z_1, z_2; \Delta x)$ or $g(z_1, z_2; \Delta x)$ do not exhibit any symmetry about the middle of the system and only show the general symmetry $\rho_2(1, 2) = \rho_2(2, 1)$, $g(1, 2) = g(2, 1)$ or $\rho_2(z_1, z_2; \Delta x) = \rho_2(z_2, z_1; \Delta x)$, $g(z_1, z_2; \Delta x) = g(z_2, z_1; \Delta x)$.

4. The gradient expansion

The density functional theory starts from the observation that all average equilibrium quantities such as density, local susceptibility, two-point distribution function, etc are functionals of the external field $(-\beta u^{\text{ext}}(\boldsymbol{r}))$. As explained in Evans (1979) one may use the relation between $\rho(\boldsymbol{r})$ and $-\beta u^{\text{ext}}(\boldsymbol{r})$ to eliminate $-\beta u^{\text{ext}}(\boldsymbol{r})$. Then all other quantities become functionals of $\rho(\boldsymbol{r})$ (in our case they depend on values of $\rho(\boldsymbol{r})$ at all points of the lattice, $\boldsymbol{r}_i$). One can try to introduce a local dependence on ρ and its spatial derivatives at any chosen point $\boldsymbol{r}$. This results from the Taylor series expansion of $\rho(\boldsymbol{r} + \Delta\boldsymbol{r})$ about $\rho(\boldsymbol{r})$. Such gradient expansions for a fluid interface have been well known since the work of van der Waals (Rowlinson and Widom 1982, Davis and Scriven 1982, Kayser and Raveche 1983). In this approach, equilibrium quantities in the interface become functions of $\rho(z)$ and its spatial derivatives $\rho' = \mathrm{d}\rho/\mathrm{d}z$, $\rho'' = \mathrm{d}^2\rho/\mathrm{d}z^2, \ldots$. We have discussed elsewhere (Stecki and Dudowicz 1985a) various interpolations of the two-point density-density distribution function across the interface and have come to the conclusion that the dependence on ρ' cannot be neglected. Here we extract this dependence from our numerical results obtained for the SOS model ($d = 2$) in various external fields and for various strip widths.

In any lattice model the gradient ρ' does not exist and we introduce the finite difference

$$\Delta\rho(z) = \tfrac{1}{2}[\rho(z-1) - \rho(z+1)] \qquad z \text{ integer} \tag{4.1}$$

unambiguously associated with point z, and the second finite difference

$$\Delta\Delta\rho(z) = \rho(z-1) + \rho(z+1) - 2\rho(z). \tag{4.2}$$

Let us consider first the distribution function $\langle\sigma\sigma\rangle$ in the central layer $z = z_{\text{mid}} = \frac{1}{2}(M+1)$ for which $\rho(z) = 0.5$ and $\Delta\Delta\rho(z) = 0$. Any variation of $\langle\sigma\sigma\rangle$ must then be ascribed to the changes of $\Delta\rho$. Figure 1 shows the computed values of $\langle\sigma\sigma\rangle$ for $\Delta x = 1$-5 against $|\Delta\rho|$ calculated from the known density profiles for strip widths $M = 29$, 21 and 11 and for external field $0.0001 \leqslant \beta_c u_0 \leqslant 0.14$ (see (3.1) and (3.2)). The plots are almost linear and extrapolate clearly to unity for $\Delta\rho = 0$, which is the value of $\langle\sigma\sigma\rangle$ in either SOS homogeneous phase. A striking feature is that points corresponding to different sizes of strips and different external fields all fall on a common line. Thus we have already obtained a striking confirmation of the ideas of the density functional theory

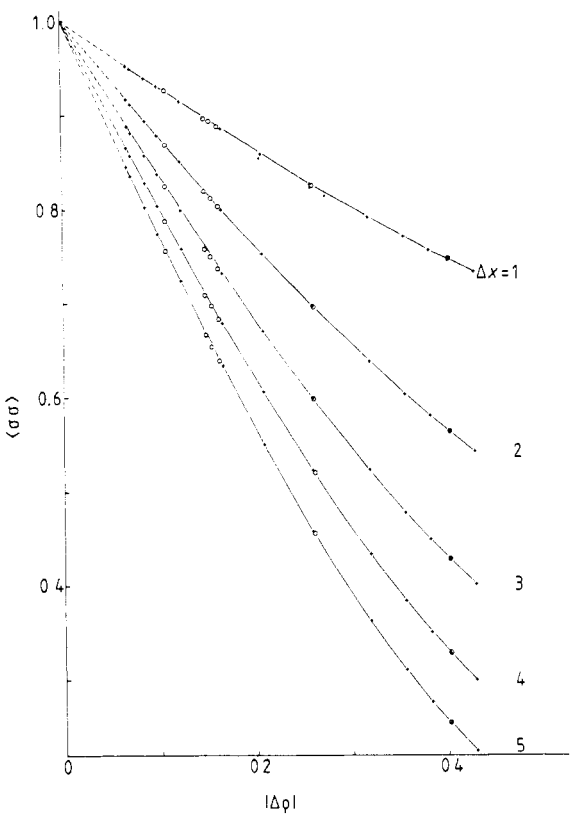

Figure 1. The in-layer distribution function $\langle\sigma\sigma\rangle_{\Delta x}$ at $z = z_{\text{mid}} = z_1 = z_2 = \frac{1}{2}(M+1)$, $\Delta x = 1$-5 for various SOS strips ($11 \leqslant M \leqslant 29$) in various external fields ($0.0001 \leqslant \beta_c u_0 \leqslant 0.14$) at $T = 0.5\ T_c$, plotted against $|\Delta\rho| = \frac{1}{2}|\rho(z+1) - \rho(z-1)|$. Circles correspond to $M = 11$ and 21, crosses to $M = 29$. For a comparison, lattice gas model with $M = 7$ and 11 is also included (dots).

since ρ, $\Delta\rho$, and $\Delta\Delta\rho$ as independent variables determine uniquely our dependent quantity $\langle\sigma\sigma\rangle$. Such a picture was found at $T = 0.5\ T_c$ (figure 1) and also at $T = 0.3\ T_c$ (figure 2).

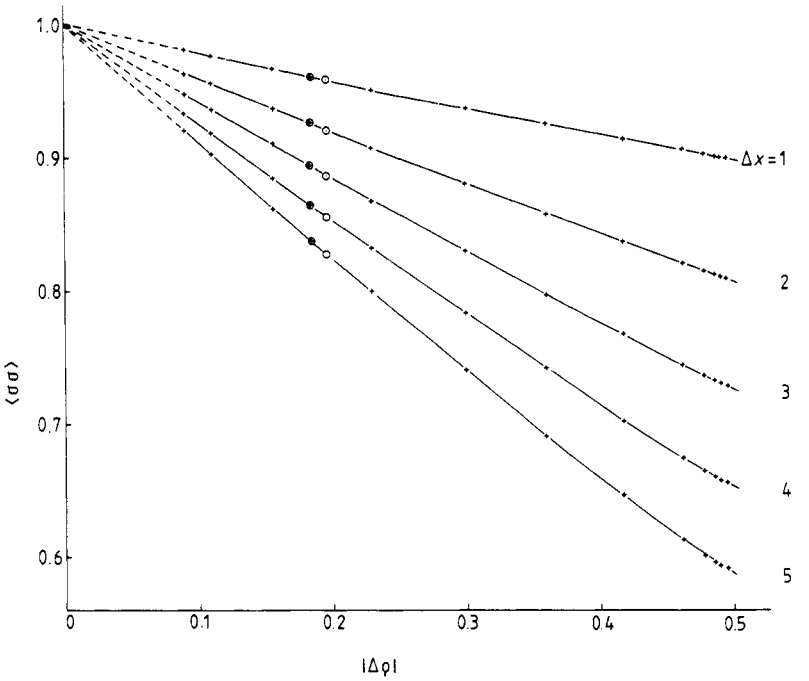

Figure 2. Same as figure 1, $T = 0.3\ T_c$. Crosses correspond to $M = 29$, circles to $M = 11, 21$.

If we consider all layers z, $z_1 = z_2 = z$, with various densities $0 < \rho(z) < 1$, the in-layer distribution function $\langle\sigma\sigma\rangle$ for $z = z_1 = z_2$ should form a surface $\langle\sigma\sigma\rangle = f(\rho, \Delta\rho, \Delta\Delta\rho, \ldots)$. As a first approximation a surface $\langle\sigma\sigma\rangle = f(\rho, \Delta\rho)$ may be considered. The relevant data are shown in figures 3 and 4 for $\Delta x = 1$ and $M = 29$. Points connected by broken lines correspond to the same value of the external field. For a given density $\rho_{\text{mod}} = \rho_0$ ($\rho_{\text{mod}} = \rho - 0.5$), $\langle\sigma\sigma\rangle_{\Delta x=1}$ decreases with $|\Delta\rho|$ and for a given $\Delta\rho$, $\langle\sigma\sigma\rangle_{\Delta x=1}$ increases with $|\rho_{\text{mod}}|$. It seems that the surface $\langle\sigma\sigma\rangle = f(|\rho_{\text{mod}}|, |\Delta\rho|)$ is reasonably smooth and unique. This observation, in connection with the universal dependence on $\Delta\rho$ of the central layer distribution function $\langle\sigma\sigma\rangle$ (see figures 1 and 2) confirms the existence of a representation of $\langle\sigma\sigma\rangle$, which we may take to be a polynomial if we are to believe the gradient theory (Davis and Scriven 1982). In our case it may be a polynomial of density ρ_{mod} and $\Delta\rho$, $\Delta\Delta\rho, \ldots$. The validity and accuracy of different polynomial representations is unknown. We can only compare which polynomials give the best fit to the existing data. For this comparision we use the least-squares method; it is described below for our case.

As a first step, polynomials in two variables ρ_{mod} and $\Delta\rho$, of the form

$$\langle\sigma\sigma\rangle_{\Delta x=1} = 1 + \sum_{k=1}^{N} a_{0k}|\Delta\rho|^k + \sum_{j\ \text{even}} \sum_{\substack{k=1 \\ j+k\leq N}} a_{jk}\rho_{\text{mod}}^j|\Delta\rho|^k \tag{4.3}$$

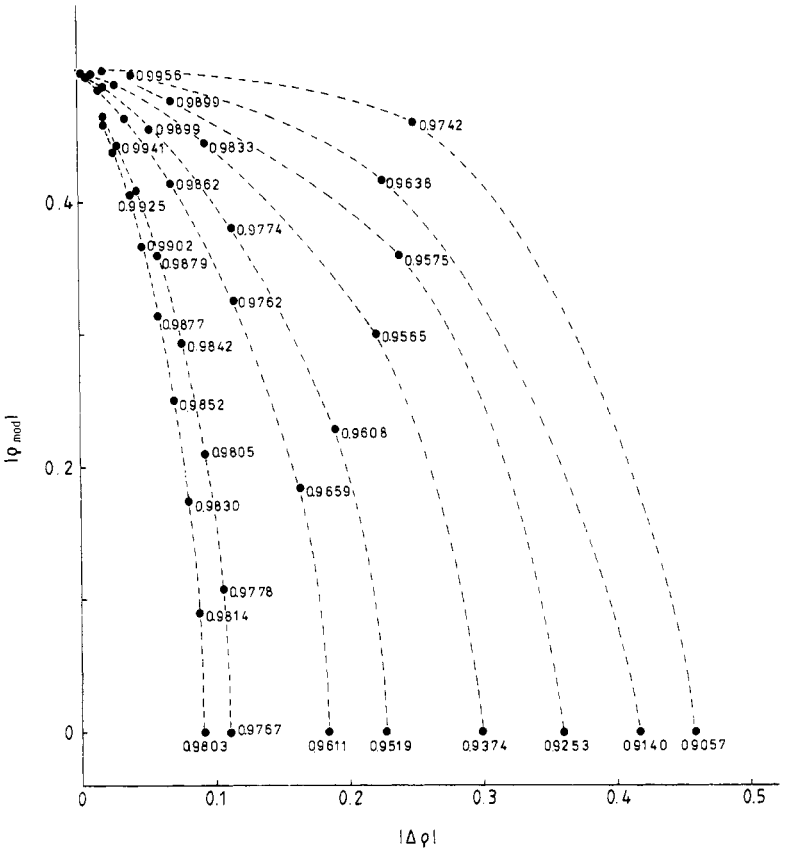

Figure 3. The in-layer distribution function $\langle\sigma\sigma\rangle$ in transverse direction $z = z_1 = z_2$, $\Delta x = 1$, as a function of two variables $|\rho_{\text{mod}}(z)| = |\rho(z) - 0.5|$ and $|\Delta\rho(z)| = \frac{1}{2}|\rho(z+1) - \rho(z-1)|$, for $M = 29$ in various external fields ($0.0001 \leq \beta_c u_0 \leq 0.14$) at $T = 0.5\ T_c$. Broken curves connect points corresponding to the same value of $\beta_c u_0$.

were applied to 115 data points representing $\langle\sigma\sigma\rangle_{\Delta x=1}$ at $T = 0.5\ T_c$. The coefficients a_{jk} found for various degrees N of the polynomial (4.3) are collected in table 1 where the values of standard deviation s_N are also given. The standard deviation s_N is defined as

$$s_N = \left(\frac{1}{n-m} \sum_{i=1}^{n} |\langle\sigma\sigma\rangle_i^{\text{calc}} - \langle\sigma\sigma\rangle_i^{\text{fit}}|^2 \right)^{1/2} \tag{4.4}$$

where n is the number of points and m—the number of constants (coefficients a_{jk}). The assumed form (4.3) requires an explanation. The terms $a_j \rho_{\text{mod}}^j$ do not occur in (4.3) since it should also describe for $\Delta\rho = 0$ the two-phase homogeneous system in which $\langle\sigma\sigma\rangle = 1$ for all proportions of two phases. In the mixed products $a_{jk}\rho_{\text{mod}}^j |\Delta\rho|^k$ only those with j even are invariant (in the range $-0.5 < \rho_{\text{mod}} < 0.5$) with respect to the change of sign $\rho_{\text{mod}} \to -\rho_{\text{mod}}$. In (4.3) we include all $1 \leq k \leq N$, because the symmetry argument which dictates a restriction to even powers of $\Delta\rho$ (Davis and Scriven 1982, Rowlinson and Widom 1982) does not apply here. We found that the fit of $\langle\sigma\sigma\rangle_{\Delta x=1}$ becomes very poor if the polynomial is so restricted (see table 1). The necessity of

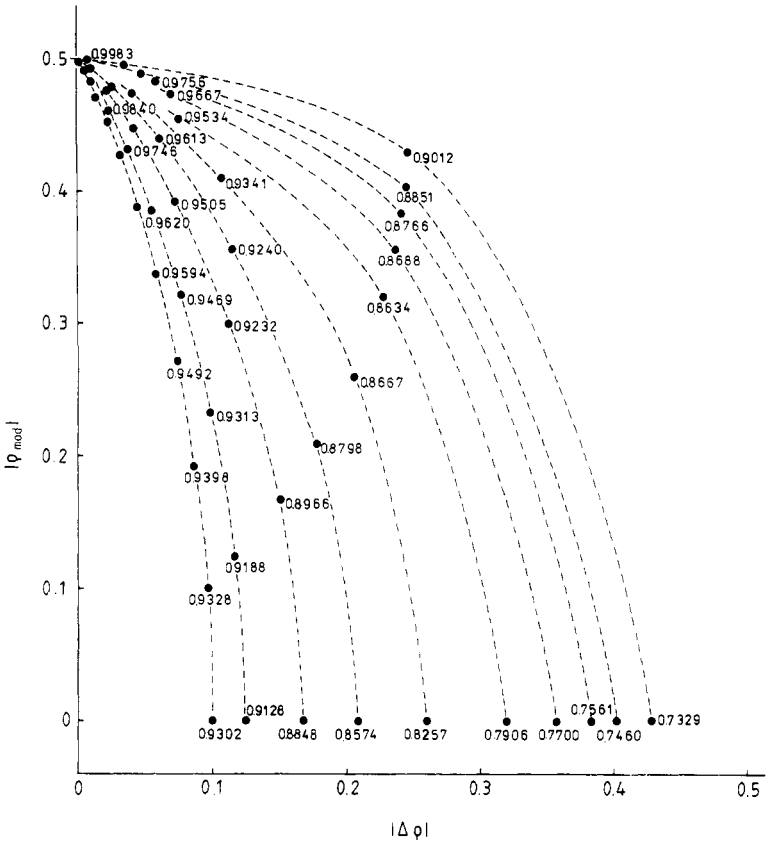

Figure 4. Same as figure 3, $T = 0.3\ T_c$.

Table 1. The coefficients a_{jk} of polynomials of degree N ($N = 4, 5, 6$), in two variables $\rho_{\text{mod}} = \rho(z) - 0.5$ and $|\Delta\rho(z)| = \frac{1}{2}|\rho(z+1) - \rho(z-1)|$, found by least-squares method applied to 115 values of distribution function $\langle\sigma\sigma\rangle_{\Delta x=1}$ at $T = 0.5\ T_c$. The standard deviations s_N are also given. For a comparison, standard deviations s_N^* corresponding to restricted polynomials (with even k only) are included. The indices j, k denote the powers of ρ_{mod} and $|\Delta\rho|$, respectively.

a_{jk}	$N = 3$	$N = 4$	$N = 5$	$N = 6$
a_{01}	−0.833 609	−0.713 067	−0.715 77	−0.808 710
a_{02}	0.888 251	−0.370 850	0.371 231	3.302 76
a_{03}	−0.948 099	2.728 99	−2.260 61	−32.359 2
a_{04}		−3.200 56	7.394 20	144.537
a_{05}			−7.022 84	−292.788
a_{06}				222.326
a_{21}	1.129 32	0.399 830	−1.452 23	−1.336 56
a_{22}		3.716 78	7.351 73	4.108 42
a_{23}			−6.585 38	9.628 16
a_{24}				−0.000 6558
a_{41}			8.089 38	9.188 99
a_{42}				−11.380 3
s_N	$0.321\,7 \times 10^{-2}$	$0.278\,9 \times 10^{-2}$	$0.142\,8 \times 10^{-2}$	$0.141\,4 \times 10^{-2}$
s_N^*		$1.934\,3 \times 10^{-2}$	$1.934\,3 \times 10^{-2}$	$1.131\,2 \times 10^{-2}$

admitting the linear term ($k = 1$) in $|\Delta\rho|$ is already apparent from figures 1 and 2 where it is clearly dominant.

Comparing table 1 and table 2, one can see that already polynomials (4.3) of two variables (table 1) reproduce $\langle\sigma\sigma\rangle_{\Delta x=1}$ very well. The standard deviation s for $N = 6$ is slightly smaller than for $N = 5$ but the coefficients vary too much to be trusted. The case with $N = 5$ seems to be the best. The simplest try with a polynomial of the third degree, $N = 3$, is already good with s about twice that for $N = 5$ or 6.

Table 2. The coefficients a_{jkl} of polynomials in three variables: $\rho_{\text{mod}}(z)$, $|\Delta\rho(z)|$ and $\Delta\Delta\rho(z) = \rho(z+1) + \rho(z-1) - 2\rho(z)$, of degree N ($N = 2, 3, 4$), obtained by least-squares fitting of the distribution function $\langle\sigma\sigma\rangle_{\Delta x=1}$ at $T = 0.5\ T_c$. The standard deviations s_N are also given.

a_{jkl}	$N=2$	$N=3$	$N=4$
a_{010}	−0.741 303	−0.707 279	−0.715 770
a_{020}	0.272 391	0.061 744	0.130 007
a_{030}		0.322 275	0.138 637
a_{040}			0.164 310
a_{002}	0.096 128	0.575 791	−8.599 49
a_{004}			−6.320 46
a_{210}		−0.297 880	−0.265 899
a_{220}			10.849 3
a_{101}	−0.322 237	−0.459 022	0.353 052
a_{103}			14.458 4
a_{202}			47.491 5
a_{301}			−3.194 00
a_{012}		−0.180 023	−26.134 3
a_{022}			34.721 7
a_{111}		1.594 63	11.379 0
a_{121}			−138.594
s_N	$1.212\,5 \times 10^{-3}$	$0.447\,2 \times 10^{-3}$	$0.173\,2 \times 10^{-3}$

In the next step, the polynomial in three variables ρ_{mod}, $\Delta\rho$ and $\Delta\Delta\rho$, of the following form

$$\langle\sigma\sigma\rangle_{\Delta x=1} = 1 + \sum_{k=1}^{N} a_{0k0}|\Delta\rho|^k + \sum_{l\ \text{even}}^{N} a_{00l}\Delta\Delta\rho^l + \sum_{j\ \text{even}} \sum_{k=1} a_{jk0}\rho_{\text{mod}}^j|\Delta\rho|^k + \sum_{\substack{j=1 \\ (j+l)\ \text{even} \\ j+l\leqslant N}} \sum_{l=1} a_{j0l}\rho_{\text{mod}}^j\Delta\Delta\rho^l + \sum_{\substack{k=1 \\ k+l\leqslant N}} \sum_{l\ \text{even}} a_{0kl}|\Delta\rho|^k\Delta\Delta\rho^l + \sum_{\substack{j=1 \\ (j+l)\ \text{even} \\ j+k+l\leqslant N}} \sum_{k=1} \sum_{l=1} a_{jkl}\rho_{\text{mod}}^j|\Delta\rho|^k\Delta\Delta\rho^l \tag{4.5}$$

was tried for fitting the same set of data points ($\langle\sigma\sigma\rangle$ for $\Delta x = 1$ at $T = 0.5\ T_c$). Table 2 contains the coefficients a_{jkl} and the standard deviations found. Similarly as in (4.3) the terms $a_{j00}\rho_{\text{mod}}$ do not occur in (4.5) for the same reason. All other terms denoted generally $\rho_{\text{mod}}^j|\Delta\rho|^k\,\Delta\Delta\rho^l$ with $j, k, l = 0, 1, 2, \ldots N (j + k + l \leqslant N)$ are taken into account

provided that the sum $(j+1)$ is even, ensuring the symmetry of $\langle\sigma\sigma\rangle$ (see (3.5)). Introducing the second finite difference $\Delta\Delta\rho$ improves the fitting.

The third degree polynomial in ρ_{mod}, $\Delta\rho$, $\Delta\Delta\rho$ describes $\langle\sigma\sigma\rangle_{\Delta x=1}$ with average accuracy of about 0.05%. The same procedure (i.e. least-squares method) was used to fit the distribution function $\langle\sigma\sigma\rangle_{\Delta x=1}$ at $T=0.3\ T_c$. The standard deviations are of the same order as those for $T=0.5\ T_c$ and also inclusion of the second finite-difference terms leads to a much better accuracy. The attempt of a simultaneous fitting of all $\langle\sigma\sigma\rangle_{\Delta x=1}$ corresponding to both temperatures $T=0.5\ T_c$, $0.3\ T_c$ failed; it means that besides the dependence on ρ_{mod}, $\Delta\rho$, $\Delta\Delta\rho$ there is a strong dependence on temperature. Therefore the coefficients are strong functions of temperature.

5. Discussion

When examining the dependence on local gradients and local density, we decided to study the distribution function $\langle\sigma\sigma\rangle$ rather than the distribution function g (or ρ_2), because $\langle\sigma\sigma\rangle$ exhibits the particle-hole symmetry of our system. Due to this property, it is sufficient to consider one half of the strip with the central layer included.

First, for $\rho=0.5$, we found a strong and almost linear dependence of $\langle\sigma\sigma\rangle$ on $|\Delta\rho|$, which extrapolated to $\Delta\rho=0$ gives the correct value of $\langle\sigma\sigma\rangle$. Different sizes of the system and different external fields produced a common curve for a given Δx. Hence we admitted the linear term in $|\Delta\rho|$ in the polynomial representation of $\langle\sigma\sigma\rangle_{\Delta x=1}$; this is correct because the symmetry arguments which impose even powers of ρ' do not apply to $\Delta\rho$. Omitting odd powers of $\Delta\rho$ in (4.3) and (4.5) leads to very poor fits of $\langle\sigma\sigma\rangle_{\Delta x=1}$.

When we consider $\langle\sigma\sigma\rangle$ for all layers, the second finite difference $\Delta\Delta\rho$ (which is zero for the central layer) should appear as an additional independent variable. And indeed, introducing $\Delta\Delta\rho$ into the polynomial improves the accuracy of description of $\langle\sigma\sigma\rangle_{\Delta x=1}$ by about one order of magnitude (see tables 1 and 2).

The dependence on the finite differences is non-analytical. For the given strip width M, the derivative $\partial\langle\sigma\sigma\rangle/\partial|\Delta\rho|$ may be written as

$$\frac{\partial\langle\sigma\sigma\rangle}{\partial|\Delta\rho|}=\frac{\partial\langle\sigma\sigma\rangle}{\partial(\beta u_0)}\frac{\partial(\beta u_0)}{\partial|\Delta\rho|}. \tag{5.1}$$

In spite of the fact that $\partial\langle\sigma\sigma\rangle/\partial(\beta u_0)$ and $\partial|\Delta\rho|/\partial(\beta u_0)$ tend to infinity for $\beta u_0\to 0$ (see figures 5 and 6), $\lim_{\beta u_0\to 0}\partial\langle\sigma\sigma\rangle/\partial|\Delta\rho|$ is finite. If $|\Delta\rho|=A_\rho|\beta u_0|^\nu$ and $\langle\sigma\sigma\rangle=1-A_\sigma|\beta u_0|^\nu$

$$\partial\langle\sigma\sigma\rangle/\partial|\Delta\rho|=A_\sigma/A_\rho, \tag{5.2}$$

where A_σ and A_ρ are constants. For $\Delta x=1$, $z_1=z_2=z_{\text{mid}}$, we found $\nu=\frac{1}{3}$.

We employed in the polynomial representation the finite differences $\Delta\rho$ and $\Delta\Delta\rho$ as independent variables. There is also another possibility of choice of independent variables. It is known (Stecki and Dudowicz 1985b) that for $\alpha=1$ the product of the external field βu_0 and the Fourier transform $\tilde{H}(z, z_{\text{mid}}; k=0)$ equals $\rho'(z)$ in the continuous system

$$\rho'(z)=-2\beta u_0\tilde{H}(z, z_{\text{mid}}; k=0) \qquad u_0>0. \tag{5.3}$$

Therefore instead of $\Delta\rho$, one can use the RHS of (5.3) as the independent variable. This attempt was carried out but the data points $\langle\sigma\sigma\rangle_{\Delta x=1}$ for $\rho=0.5$ corresponding

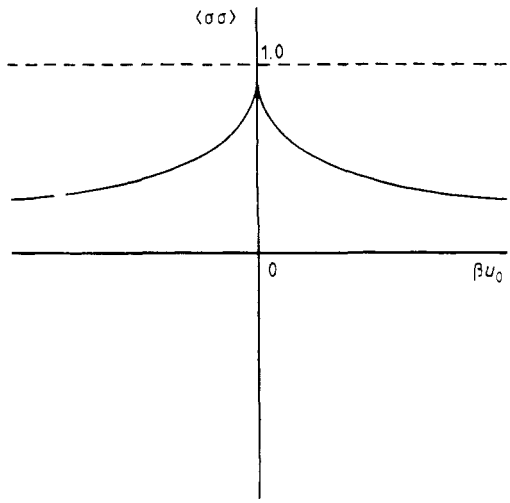

Figure 5. Typical behaviour of the SOS distribution function $\langle\sigma\sigma\rangle_{\Delta x}$ in transverse direction $z = z_{\text{mid}} = z_1 = z_2$ with external field βu_0 variable. As $\beta u_0 \to 0^+$, $\partial\langle\sigma\sigma\rangle/\partial(\beta u_0) \to -\infty$.

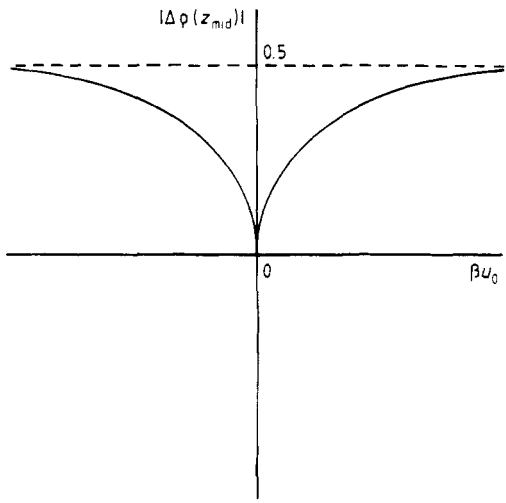

Figure 6. Typical plot of first finite difference $|\Delta\rho(z_{\text{mid}})|$ against external field βu_0. As $\beta u_0 \to 0^+$, $\partial|\Delta\rho(z_{\text{mid}})|/\partial(\beta u_0) \to \infty$.

to different strip widths and different external fields do not fall on a common line, in contrast to previously found universal dependence on $\Delta\rho$ (see figures 1 and 2).

All our results given here are related to an external field ($\alpha = 1$) determined by the step function. The case of the gravitational field ($\alpha = 2$), damping density fluctuations in the interface zone more strongly, has not been examined yet. We suppose that the independent variables ρ, $\Delta\rho$, $\Delta\Delta\rho$ will determine the structure of interface uniquely and accurately also for the case of the gravitational field ($\alpha = 2$).

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