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LETTER TO THE EDITOR

On the field-dependence of eigenvalues of correlation function matrices H and C in the fluctuating interface of the two-dimensional SOS model

J Stecki†‡ and J Dudowicz‡

† Physical Chemistry Laboratory, Oxford, South Parks Road, UK
‡ Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Kasprzaka 48/52, Poland

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Abstract. The density–density correlation function matrix $H(z_1, z_2; x)$ and its Fourier transform $\tilde{H}(z_1, z_2; k)$ in the interface of a lattice gas in the solid-on-solid (SOS) approximation were computed numerically with the aid of the transfer matrix. Strips $z_{\max} \times \infty$ were studied in a weak external field. The matrices H and $\tilde{H}$ were diagonalised for small $k_\perp$ and for $k_\perp = 0$. As postulated by Wertheim, the largest (single) eigenvalue of $\tilde{H}(k_\perp = 0)$ was well separated from the others, but its field dependence was represented by $\lambda_H^{-1} = A(\beta V_0)^\delta$ with $\delta = 0.75$ or $\delta = 1$ for $\alpha = 2$ or $\alpha = 1$ respectively, with α specifying the power law of the external field.

The structure of the fluctuating interface between two fluid phases in a gravitational field is conventionally described by the density profile $\rho(z)$ and by the two-point density–density correlation function $H(1, 2) = \langle \delta\rho(1)\, \delta\rho(2) \rangle$. H contains the long-range transverse correlations and the universal form representing the 'capillary wave' contribution is

$$\tilde{H}(z_1, z_2; k_\perp) = \tilde{H}(z_1, z_2; k_\perp = 0) \cdot \beta mg\, \Delta\rho / (\beta mg\, \Delta\rho + \beta\gamma k_\perp^2) \qquad k_\perp \to 0 \tag{1a}$$

$$\tilde{H}(0) \equiv \tilde{H}(z_1, z_2; k_\perp = 0) = \rho'(z_1)\rho'(z_2)/\beta mg\, \Delta\rho \qquad \rho'(z) = \mathrm{d}\rho/\mathrm{d}z \tag{1b}$$

with the external potential $\beta V(z) = \beta mg(z - z_0)$, $\Delta\rho = \rho_{\text{gas}} - \rho_{\text{liq}}$, $\beta = 1/kT$, γ being the surface tension and $k_\perp$ the transverse Fourier variable (Rowlinson and Widom 1982, Evans 1979 (especially appendix 2), Croxton 1980, Davis and Scriven 1982). The long range of $H(x)$ becomes infinite in the limit of $\beta mg \to 0$. These results follow from a one-eigenvalue approximation to $\tilde{H}$.

Having computed numerically for a certain model, the matrices $\tilde{H}(k)$ and their inverses $\tilde{C}(k)$ (Stecki 1984, Dudowicz and Stecki 1980) we can test the ansatz proposed by Wertheim (1976) and discussed by Evans (1979). Wertheim found that $\rho'(z)$ is an eigenfunction of $C(k_\perp = 0)$ with an eigenvalue zero if $\beta mg = 0$ and postulated that this smallest eigenvalue of $C, \lambda_0(k, \beta mg)$ goes to zero linearly, i.e. $\lambda_C(0, \beta mg) = \beta mg\nu$, $\beta mg \to 0$, ν finite.

We studied the SOS model in two dimensions which replaces the interface by an array of columns of liquid ($\rho_L = 1$) of variable height h_i, in contact with vacuum ($\rho_G = 0$). The matrices H and C are readily computed (Stecki 1984) with the aid of the transfer matrix for non-zero external (pinning) potential $V(h_i) = V_0|h_i - h_0|^\alpha$ (van Leeuwen and

Hilhorst 1981). We studied the case $\alpha = 2$ which corresponds to a gravitational potential and the case $\alpha = 1$ which corresponds to constant shift, in the chemical potential, of opposite signs below and above the Gibbs dividing surface. For a strip $z_{max} = \infty$, H (or C) is a matrix of dimensions $z_{max} \times z_{max}$ and its eigenvalues were computed for $z_{max} = 11$–61 and a range of external fields $2 \times 10^{-5} \leq \beta V_0 \leq 0.3$ and temperatures $T/T_c = 0.3, 0.5, 0.7$ where $2J/kT_c = \ln(1+\sqrt{2}) = 0.881\,37$. The partition function of the system is

$$Z = \sum_{\{h_i\}} \exp\left(-2\beta J \sum_i |h_{i+1} - h_i|\right) \exp\left(\beta V_0 \sum_i |h_i - h_0|^\alpha\right), \qquad \alpha = 1, 2$$

$$0 \leq h_i \leq z_{max}. \tag{2}$$

The transfer matrix was diagonalised numerically, all its eigenvalues and eigenvectors were found and the Fourier sum $\tilde{H}(k)$ was hence computed. All eigenvalues of $\tilde{H}(k_\perp = 0)$ matrix were then found. Figure 1 shows the log–log plot of $\lambda_C = \lambda_H$ against $\beta_c V_0 = 0.881\,37\, V_0/2J$. The plot of figure 1 was obtained by extrapolating each λ_C to larger and larger values of z_{max} until it remained constant (except for the very small fields ($\beta_c V_0 < 2 \times 10^{-4}$), to five digit accuracy). Such extrapolation becomes more and more difficult as the temperature is raised.

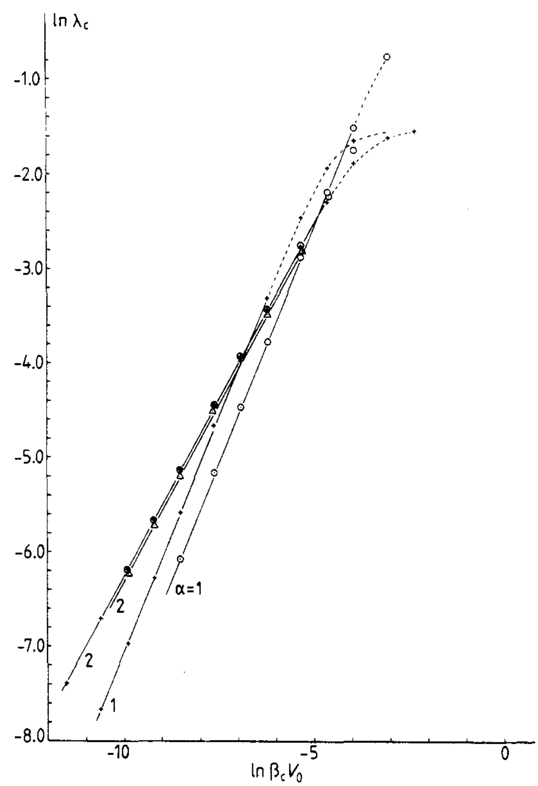

Figure 1. The log–log plot of the eigenvalue $\lambda_C(k_\perp = 0)$ against external field $\beta_c V_0$ for temperatures $T/T_c = 0.3(+)$, $0.5(\bigcirc)$, $0.7(\triangle)$. Here $\alpha = 2$ corresponds to the gravitational field, and $\alpha = 1$ corresponds to constant shift in chemical potential.

The linear plots of figure 1 correspond to the following relation

$$\lambda_C = A(T)(\beta_c V_0)^{\delta}. \tag{3}$$

We found the amplitudes and the exponents by extrapolation illustrated by figure 2. Each δ in figure 2 was obtained from a pair of successive points in figure 1. For the gravitational potential $\alpha = 2$, $\delta = \frac{3}{4}$ in the limit of vanishing external field. The exponent $\delta = 1$ postulated by Wertheim is recovered in the case $\alpha = 1$. The amplitudes are: $A = 3.50 \pm 0.01, 3.50 \pm 0.06$ for $T/T_c = 0.3, 0.5$, respectively, for $\alpha = 2$ and $A = 18.7 \pm 0.1, 11.25 \pm 0.1$ for $T/T_c = 0.3, 0.5$, respectively, for $\alpha = 1$. The amplitude could be determined for $T/T_c = 0.7$ if larger strips were investigated.

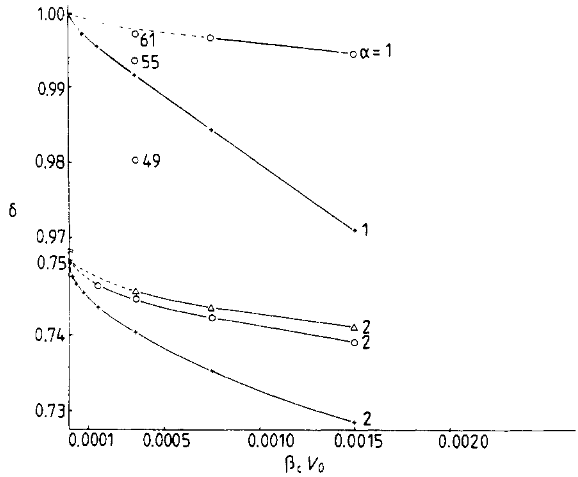

Figure 2. The exponents δ computed as successive ratios from figure 1 for $\alpha = 2$ and $\alpha = 1$. The numbers 49, 55, 61 denote z_{max} for $\alpha = 1$, $T = 0.5 T_c$. For $z_{max} = 61$ the proper value of λ_c is not yet reached.

It is worth pointing out that the result (3) does not necessarily destroy the forms $(1a)$ and $(1b)$. Assuming and introducing the one-eigenvalue approximation to H, we find (now in continuous space, Evans 1979)

$$\tilde{H} = x_1(z_1)A^{-1}(\beta_c V_0)^{-\delta}x_1(z_2)$$

$$\rho'(z_1) = -A^{-1}(\beta_c V_0)^{1-\delta}x_1(z_1)E$$

$$\Delta\rho = A^{-1}(\beta_c V_0)^{1-\delta}E^2$$

$$E \equiv \int \mathrm{d}z_1\, x_1(z_1)$$

but

$$\tilde{H} = \rho'(z_1)\rho'(z_2)(\beta mg\, \Delta\rho)^{-1} \tag{1b}$$

is recovered because δ cancels out. The k^2 dependence in $(1a)$ is confirmed as expected but the coefficient approaches $\beta\gamma$ with difficulty.

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