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The direct correlation function for an interface of a two-dimensional model in a weak gravitational field

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Abstract. The direct correlation function for a fluctuating interface in a two-dimensional solid-on-solid lattice model is studied. We obtain for a weak gravitational field an asymptotic expression for the direct correlation function that agrees well with previous numerical results. In particular two different vertical length scales appear.

1. Introduction

Physical properties of fluctuating interfaces are of importance and has recently received increasing attention (Rowlinson and Widom 1982, Bedeaux 1986, Fisher 1984). Fluctuations of the interface between two fluid phases have different character depending upon the dimensionality, and are particularly strong for low-dimensional systems. A planar interface may be maintained by a gravitational field, such that in the limit of vanishing gravity the width of the interface diverges. Since gravity is a weak force one is led naturally to consider expansions in which the gravitational constant g is assumed to be the small parameter.

In a recent article (Hemmer and Lund 1988) asymptotic results are given for a particular model—the solid-on-solid lattice gas model in two dimensions—a model which has also been studied by numerical means (Stecki and Dudowicz 1986) in the low-gravity regime. In particular, the asymptotic results derived so far include the density profile, local and global susceptibilities, as well as the density-density correlation function. The characteristic length scales involved, both along the interface and normal to the interface, diverge (in different ways) in the weak gravity limit.

For the direct correlation function it was, in contrast, found that indeed it is of short range both along the interface (Stecki 1984) and as a function of height differences (Stecki and Dudowicz 1986, Hemmer and Lund 1988). The purpose of the present paper is to study the detailed properties of the direct correlation function, and to provide explicit analytic expressions asymptotically valid for weak gravity. These properties are to some extent known from earlier numerical work by Dudowicz and Stecki (1986), and some aspects are also intimately related to a recent finite-size analytic of the same model in the absence of any external field (Ciach 1987, Ciach *et al* 1987).

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2. The model and the associated eigenvalue problem

The interface between an upper gas phase and a lower liquid phase can, in the lattice model, be described by a set (h_i) of integer heights, measured from the average height of the interface. The Hamiltonian of the two-dimensional model is of the nearest-neighbour type:

$$H = 2J \sum_{i=1}^{L} |h_i - h_{i+1}| + g \sum_{i=1}^{L} h_i^2 \tag{1}$$

where g is a measure of the gravitational field. Eventually the horizontal length $L \to \infty$.

The probability distribution $P(h_i)$ of an interface configuration is conveniently expressed in terms of a transfer matrix

$$T(h_i, h_j) = \exp(-2K|h_i - h_j| - \tfrac{1}{2}Gh_i^2 - \tfrac{1}{2}Gh_j^2) \tag{2}$$

where $K = \beta J$ and $G = \beta g$. Explicitly

$$P(\{h_i\}) = Z^{-1} \prod_{i=1}^{L} T(h_i, h_{i+1}) \tag{3}$$

with the partition function

$$Z = \sum_{\{h_i\}} \exp(-\beta H) = \sum_h (T^L)_{hh}. \tag{4}$$

All physical quantities are expressible in terms of eigenvectors ψ_n and eigenvalues λ_n of the transfer matrix:

$$T\psi_n = \lambda_n \psi_n \qquad \lambda_0 \geqslant \lambda_1 \geqslant \lambda_2 \geqslant \ldots . \tag{5}$$

For a weak gravitational field it is possible to perform an asymptotic expansion of the eigenvalues and eigenvectors (Hemmer and Lund 1988). The eigenvalues are all degenerate for zero gravity, but a weak gravitational field resolves the degeneracy:

$$\lambda_n = \coth K\{1 - (2n+1)\varepsilon + [\tfrac{11}{4}n(n+1) + \tfrac{7}{8} + \tfrac{1}{2}(n^2 + n + \tfrac{1}{2}) \sinh^2 K]\varepsilon^2 + \mathrm{O}(\varepsilon^3)\} \tag{6}$$

where

$$\varepsilon = \tfrac{1}{2}G^{1/2}/\sinh K. \tag{7}$$

The eigenfunctions are most naturally considered as functions of the scaled variable

$$y = \gamma h = G^{1/4}(2 \sinh K)^{1/2} h. \tag{8}$$

The asymptotic eigenfunction expansion also proceeds in powers of ε. To lowest order the eigenfunctions are harmonic oscillator eigenfunctions. The principal eigenfunction

$$\psi_0(h) = \gamma^{1/2}\pi^{-1/4} \exp(-\tfrac{1}{2}y^2)[1 + \varepsilon(2\sinh^2 K + 3)(\tfrac{1}{48}y^4 - \tfrac{3}{16}y^2 + \tfrac{5}{64}) + \mathrm{O}(\varepsilon^2)] \tag{9}$$

will be of particular importance below.

3. Correlation functions

The two-point height distribution function $p(h, h'; x)$ is the probability of simultaneously finding the heights $h_i = h$ and $h_{i+x} = h'$ of two columns separated by a horizontal distance x. In terms of eigenvalues and eigenvectors of the transfer matrix we have

$$p(h, h'; x) = \sum_{n=0}^{\infty} (\lambda_n/\lambda_0)^x \psi_n(h)\psi_n(h')\psi_0(h)\psi_0(h'). \tag{10}$$

For large separations x only the first term remains, and the remaining sum represents therefore the height-height *correlation* function

$$g(h, h'; x) = \sum_{n=1}^{\infty} (\lambda_n/\lambda_0)^x \psi_n(h)\psi_n(h')\psi_0(h)\psi_0(h'). \tag{11}$$

The corresponding *density-density* correlation function is therefore

$$\begin{aligned} H(z, z'; x) &= \sum_{h=z}^{\infty} \sum_{h'=z'}^{\infty} g(h, h'; x) \\ &= \sum_{h=z}^{\infty} \sum_{h'=z}^{\infty} \sum_{n=1}^{\infty} (\lambda_n/\lambda_0)^x \psi_n(h)\psi_n(h')\psi_0(h)\psi_0(h'). \end{aligned} \tag{12}$$

Introducing a discrete Fourier transform with respect to horizontal distances:

$$\tilde{H}(z, z'; k) = \sum_{x=-\infty}^{\infty} \exp(ikx) H(z, z'; x) \tag{13}$$

we have

$$\tilde{H}(z, z'; k) = \sum_{h=z}^{\infty} \sum_{h'=z'}^{\infty} \sum_{n=1}^{\infty} \psi_n(h)\psi_n(h')\psi_0(h)\psi_0(h') f_n(k) \tag{14}$$

with

$$f_n(k) = \frac{\lambda_0^2 - \lambda_n^2}{\lambda_0^2 + \lambda_n^2 - 2\lambda_0\lambda_n \cos k}. \tag{15}$$

The direct correlation function $C(z_1, z_2; x)$ is the matrix inverse of H:

$$\sum_{x_2, z_2} H(z_1, z_2; x_1 - x_2) C(z_2, z_3; x_2 - x_3) = \delta_{z_1, z_3} \delta_{x_1, x_3} \tag{16}$$

or, alternatively,

$$\sum_{z_2} \tilde{H}(z_1, z_2; k) \tilde{C}(z_2, z_3; k) = \delta_{z_1, z_3}. \tag{17}$$

A formally exact expression for $\tilde{C}$ is

$$\tilde{C}(z_1, z_2; k) = \Delta_1 \Delta_2 \sum_{n=1}^{\infty} \psi_n(z_1)\psi_n(z_2)[\psi_0(z_1)\psi_0(z_2) f_n(k)]^{-1} \tag{18}$$

introducing the difference operator Δ_1 through $\Delta_1 F(z_1, z_2) = F(z_1, z_2) - F(z_1 + 1, z_2)$, and similarly for Δ_2 (Hemmer and Lund 1988). Expression (18) is easily verified by direct insertion of (14) and (18) into the defining equation (17).

From the simple k dependence of $\tilde{C}$,

$$\tilde{C}(z_1, z_2; k) = C_0(z_1, z_2) + 2C_1(z_1, z_2) \cos k \tag{19}$$

it follows (Stecki 1984) that the direct correlation function is *strictly short-ranged* in the sense that

$$C(z_1, z_2; x) = 0 \qquad \text{for} \qquad |x| > 1. \tag{20}$$

Moreover, $C(z_1, z_2, x = 0) = C_0(z_1, z_2)$ and $C(z_1, z_2; x = \pm 1) = C_1(z_1, z_2)$. From (13), (16) and (17) we obtain

$$C_0(z_1, z_2) = \Delta_1 \Delta_2 \psi_0^{-1}(z_1)\psi_0^{-1}(z_2) \sum_{n=1}^{\infty} \frac{\lambda_0^2 + \lambda_n^2}{\lambda_0^2 - \lambda_n^2} \psi_n(z_1)\psi_n(z_2) \tag{21}$$

and

$$C_1(z_1, z_2) = -\Delta_1\Delta_2\psi_0^{-1}(z_1)\psi_0^{-1}(z_2) \sum_{n=1}^{\infty} \frac{\lambda_0\lambda_n}{\lambda_0^2-\lambda_n^2} \psi_n(z_1)\psi_n(z_2). \tag{22}$$

These exact equations form the basis for the weak-gravity asymptotic expansion. It will be convenient to express the two non-direct correlation functions C_0 and C_1 in terms of

$$c(h_1, h_2; a) = \Delta_1\Delta_2\psi_0^{-1}(h_1)\psi_0^{-1}(h_2) \sum_{n=0}^{\infty} \frac{\lambda_0+a\lambda_n}{\lambda_0-a\lambda_n} \psi_n(h_1)\psi_n(h_2). \tag{23}$$

Then

$$C_0(h_1, h_2) = \tfrac{1}{2}c(h_1, h_2; 1) + \tfrac{1}{2}c(h_1, h_2; -1) \tag{24}$$

and

$$C_1(h_1, h_2) \equiv -\tfrac{1}{4}c(h_1, h_2; 1) + \tfrac{1}{4}c(h_1, h_2; -1). \tag{25}$$

The $n=0$ term in (23) can be included since the gradient operation annihilates the extra term. It is obvious, however, that the auxiliary variable a can *not* be set equal to unity before the gradient operation is performed.

Using

$$\frac{\lambda_0+a\lambda_n}{\lambda_0-a\lambda_n} = 1 + \sum_{s=1}^{\infty} \lambda_n^s\lambda_0^{-s}a^s \tag{26}$$

orthogonality of the eigenvectors, and the eigenfunction expansion of the sth iterated transfer matrix:

$$T^{(s)}(h_1, h_2) = \sum_n \lambda_n^s\psi_n(h_1)\psi_n(h_2) \tag{27}$$

we may express (23) as

$$c(h_1, h_2; a) = \Delta_1\Delta_2\psi_0^{-1}(h_1)\psi_0^{-1}(h_2)\left(\delta_{h_1,h_2} + 2\sum_{s=1}^{\infty} (a/\lambda_0)^s T^{(s)}(h_1, h_2)\right). \tag{28}$$

So far everything is exact. We are now prepared for the weak-gravity expansion.

4. Weak-gravity expansion, lowest order

Since by (9)

$$\psi_0(h+1) = \psi_0(h)[1 + O(\sqrt{G})] \tag{29}$$

we have

$$c(h_1, h_2; a) = \psi_0^{-1}(h_1)\psi_0^{-1}(h_2)\Delta_1\Delta_2 \times\left(\delta_{h_1h_2} + 2\sum_{s=1}^{\infty} (a/\lambda_0)^s T^{(s)}(h_1, h_2)\right)[1 + O(\sqrt{G})]. \tag{30}$$

To lowest order we also replace the transfer matrix (2) by its $G=0$ version:

$$T(h_1, h_2) \to T_0(h_1, h_2) = \exp(-2K|h_1 - h_2|). \tag{31}$$

In terms of the Fourier representation

$$\exp(-2K|h-h'|)=\frac{1}{2\pi}\int_{-\pi}^{\pi}\mathrm{d}k\,\exp(-\mathrm{i}k(h-h')]\frac{\sinh 2K}{\cosh 2K-\cos k} \tag{32}$$

the sth iterated kernel of T_0 is trivially

$$T_0^{(s)}(h_1-h_2)=\frac{1}{2\pi}\int_{-\pi}^{\pi}\mathrm{d}k\,\exp[-\mathrm{i}k(h_1-h_2)]\left(\frac{\sinh 2K}{\cosh 2K-\cos k}\right)^s. \tag{33}$$

Inserting into (30), summing the geometric series, and using

$$\Delta_1\Delta_2\exp[-\mathrm{i}k(h_1-h_2)]=\exp[-\mathrm{i}k(h_1-h_2)]2(1-\cos k) \tag{34}$$

we have, to dominating order,

$$c(h_1,h_2;a)=\psi_0^{-1}(h_1)\psi_0^{-1}(h_2)\times\left(\Delta_1\Delta_2\delta_{h_1,h_2}+\frac{2a\sinh 2K}{\pi\lambda_0}\int_{-\pi}^{\pi}\mathrm{d}k\frac{(1-\cos k)\exp[-\mathrm{i}k(h_1-h_2)]}{\cosh 2K-a\lambda_0^{-1}\sinh 2K-\cos k}\right). \tag{35}$$

We also insert the lowest-order approximation for the eigenvalue:

$$\lambda_0\rightarrow\lambda_0^{(0)}=\coth K \tag{36}$$

see (6). This gives

$$c(h_1,h_2;1)=\psi_0^{-1}(h_1)\psi_0^{-1}(h_2)(\Delta_1\Delta_2-8\sinh^2 K)\delta_{h_1h_2} \tag{37}$$

and

$$\begin{aligned}c(h_1,h_2;-1)&=\psi_0^{-1}(h_1)\psi_0^{-1}(h_2)\\&\quad\times\left(\Delta_1\Delta_2\delta_{h_1,h_2}+4\pi^{-1}\sinh^2 K\int_{-\pi}^{+\pi}\mathrm{d}k\frac{(1-\cos k)\exp[-\mathrm{i}k(h_1-h_2)]}{1+4\sin^2 K-\cos k}\right)\\&=\psi_0^{-1}(h_1)\psi_0^{-1}(h_2)\left((\Delta_1\Delta_2-8\sinh^2 K)\delta_{h_1,h_2}+\frac{32\sinh^4 K}{\sinh B_0}\exp(-B_0|h_1-h_2|)\right)\end{aligned} \tag{38}$$

where the positive quantity B_0 is related to K via

$$\cosh B_0=1+4\sinh^2 K \tag{39}$$

or, alternatively,

$$\sinh\tfrac{1}{2}B_0=\sqrt{2}\sinh K. \tag{40}$$

Inserting (37) and (38) into (24) and (25) we have, to lowest order,

$$C_0(h_1,h_2)=\psi_0^{-1}(h_1)\psi_0^{-1}(h_2)\times\left[2\delta_{h_1,h_2}-\delta_{h_1-1,h_2}-\delta_{h_1,h_2-1}+\frac{16\sinh^4 K}{\sinh B_0}\exp(-B_0|h_1-h_2|)\right] \tag{41}$$

and

$$C_1(h_1,h_2)=\psi_0^{-1}(h_1)\psi_0^{-1}(h_2)\times\left(-4\sinh^2 K\,\delta_{h_1,h_2}+\frac{8\sinh^4 K}{\sinh B_0}\exp(-B_0|h_1-h_2|)\right). \tag{42}$$

The functions in brackets in (41) and (42) become rapidly negligible when the difference between the heights h_1 and h_2 increases. The prefactor, however, is slowly varying and is therefore effectively a function of the average height:

$$C^{lr}(h_1, h_2) = \psi_0^{-1}(h_1)\psi_0^{-1}(h_2) \simeq \psi_0^{-2}(\tfrac{1}{2}h_1 + \tfrac{1}{2}h_2)$$
$$\simeq \gamma^{-1}\sqrt{\pi}\exp[\gamma^2(h_1+h_2)^2/4]. \qquad (43)$$

This completes the derivation of the direct correlation function for weak gravity. The final results $C_0(h_1, h_2)$ and $C_1(h_1, h_2)$ as given by (41) and (42) agree excellently with the numerical computations reported by Stecki and Dudowicz and (1986) and their analysis of them.

5. The field dependence of the intrinsic correlation length

The lowest-order expressions (41) and (42) show that the short-range correlations for $|h_1 - h_2| > 1$ consists of an exponentially decaying function of the height difference, with an inverse intrinsic correlation length B_0. Will the intrinsic correlation length increase or decrease when the gravitational field increases? In order to answer this question we now compute the inverse intrinsic correlation length to next order, i.e. to $O(\sqrt{G})$.

The exponential function originates from the sum $c(h_1, h_2; 1)$, (28). Replacing the exact transfer matrix $T(h_1, h_2)$, (2), by $T_0(h_1, h_2) = \exp(-2K|h_1 - h_2|)$, we make an error of $O(G)$ only. To order $\sqrt{G}$, then, the iterated kernels take the form (33), the geometric series can be summed and the Fourier transform taken. The result is

$$c(h_1, h_2; -1) = -\Delta_1\Delta_2 \frac{A\exp(-B|h_1 - h_2|)}{\psi_0(h_1)\psi_0(h_2)} \qquad (44)$$

with A and B defined through

$$\cosh B = \cosh 2K + \lambda_0^{-1}\sinh 2K \qquad (45)$$

and

$$A = \frac{2\sinh 2K}{\lambda_0 \sinh B}. \qquad (46)$$

Using in (45) the expansion (8) of the principal eigenvalue λ_0, we obtain to $O(\sqrt{G})$

$$\cosh B = 1 + 4\sinh^2 K + \sqrt{G}\sinh K. \qquad (47)$$

Introducing the zeroth-order inverse correlation length B_0, (39), we can express B, consistently to $O(\sqrt{G})$, as

$$B = B_0 + B_1\sqrt{G} = B_0 + \sqrt{G}\frac{\sinh K}{\sinh B_0} \qquad (48)$$

We see that B increases with G, and this answers the question posed above: the intrinsic correlation length *decreases* with increasing field.

Stecki and Dudowicz (1986) studied the field dependence of the intrinsic correlation length in a different way. They considered the direct correlation functions C_0 and C_1

for several height differences $d = h_1 - h_2 > 1$, always *at* the interface, i.e. $h_1 + h_2 = 0$ or 1 (depending upon whether d is even or odd). The quantity

$$\tilde{B} = \ln\left(\frac{C_i(d_1)}{C_i(d_2)}\right)^{1/(d_2-d_1)} \tag{49}$$

would be a (field-dependent) constant if the direct correlation function $C_i(d)$, $i = 0$ or 1, were decaying exponentially with the height difference.

Using their very precise numerical values for the correlation functions they obtained for several sets (d_1, d_2) the field dependence of $\tilde{B}$ (figure 1). With Dudowicz and Stecki we note three main features.

(i) The straight lines show that a $\sqrt{G}$ effect is seen.

(ii) For $G = 0$ all values $\tilde{B}$ converge to a common value, which agrees numerically with B_0 of (39).

(iii) There *is* a dependence on d_1 and d_2.

Since we just have determined the relevant part the short-range direct correlation function to order $\sqrt{G}$, it is easy to obtain the weak field expansion of $\tilde{B}$ to this order.

The direct correlation functions in this range are, by (44), proportional to

$$C_i(h_1, h_2) \propto \Delta_1\Delta_2 \frac{\exp(-B|h_1 - h_2|)}{\psi_0(h_1)\psi_0(h_2)}. \tag{50}$$

The operation $\Delta_1\Delta_2$ produces four terms. By inserting the lowest-order expression (9) for ψ_0, expressing C_i in terms of the difference $d = h_1 - h_2$, assuming $h_1 + h_2 = 0$ or 1, expanding consistently in $\sqrt{G}$, and inserting into (49), we obtain the result

$$\tilde{B}(d_1, d_2) = B_0 + \tfrac{1}{2}\sinh K(2/\sinh B_0 + 2\coth\tfrac{1}{2}B_0 - d_1 - d_2)\sqrt{G} \tag{51}$$

to this order. (When d_1 is odd and d_2 even, or vice versa, a factor $\exp(\gamma^2/4)$, originating from the long-range part C^{lr} of the direct correlation function, is present. This factor is included neither in (51) nor in figure 1.) The analytic result (51) is in excellent agreement with the numerical results in figure 1.

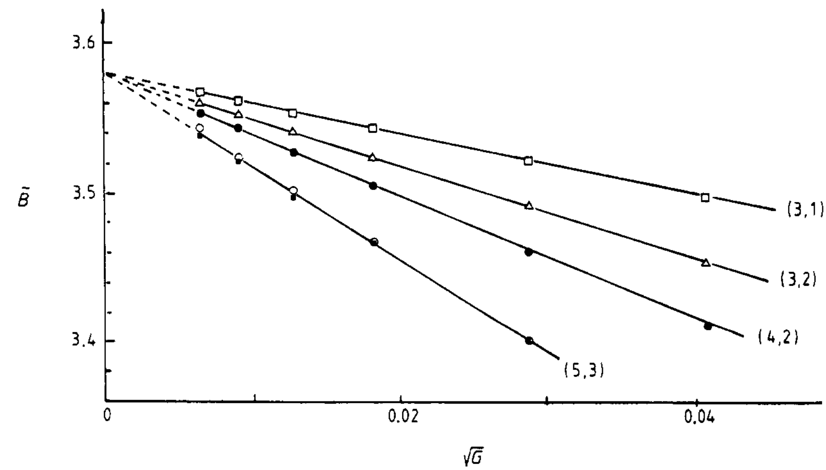

Figure 1. The function $\tilde{B}$, (49), determined from ratios of numerically exact direct correlation functions $C(d_1)/C(d_2)$, as a function of the gravitational field. The values (d_1, d_2) of the height differences are given. The temperature is $0.3\,T_c$ ($K = 1.968\,956$). (From Stecki and Dudowicz 1986.)

6. Discussion

We have shown above how to execute a weak-field asymptotic analysis of the direct correlation function $C(h_1, h_2; \Delta x)$ for the present two-dimensional system.

The direct correlation function has some remarkable properties: it is short-ranged in its dependence upon Δx, the distance along the interface; in our model strictly short-ranged in the sense that $C=0$ beyond a certain distance (here beyond $\Delta x = 1$). Thus the second moment of C, needed in the Yvon–Triezenberg–Zwanzig expression for the surface tension becomes simply $2C_1$ in this model.

The dependence of C on the height variables h_1 and h_2 appears in two very different ways. To dominating order in the asymptotic analysis the direct correlation function consists of two factors:

$$C(h_1, h_2; \Delta x) = C^{lr}(h_1, h_2) C^{sr}(h_1, h_2; \Delta x). \tag{52}$$

The short-ranged factor C^{sr} is a function of relative heights $|h_1 - h_2|$ and becomes quickly negligible with increasing height differences. This is physically reasonable when the relevant horizontal distances never exceed 1. The long-ranged factor $C^{lr}(h_1, h_2)$, seen as $\psi_0^{-1}(h_1)\psi_0^{-1}(h_2)$ in (41) and (42), is a function of scaled variables and varies on the scale of the large interface width. Since the short-ranged factor requires the heights h_1 and h_2 to be essentially equal on this scale, the long-ranged factor can be considered to depend on one variable, the average height. It is tempting to interpret the long-range factor to represent capillary wave fluctuations, while the short-range factor contains detailed information about the short-range structure of the interface.

It is interesting to make contact with the work of Ciach (1987) who studied the same model with no gravitational field, but with a large finite size M in the vertical direction. The finite size M prevents, in a roughly similar way as a finite G, divergent interface fluctuations. Ciach found, for $M \to \infty$, a short-range factor in the direct correlation function, Stecki and Dudowicz (1986) realised that their numerical values agreed well with the Ciach short-range factor, and, indeed, our results in section 4 verify that the lowest-order short-range functions $C^{sr}(h_1, h_2; \Delta x)$ for the two models are identical.

Considerable care must be exercised in the asymptotic analysis. The gradient operators in the exact expression (28) produce four terms, and we have argued that gradients of the ψ_0^{-1} factors produce terms of higher order in the small parameter G and should not be carried along. However, by themselves these additional terms would diverge when the auxiliary variable $a \to 1$ (see also Dudowicz 1988). The proper procedure is to collect all terms of a given order in G (also those arising from the dominant contribution that we kept) before we set $a = 1$. This is, however, not an easy task because it is non-trivial to iterate the transfer matrix beyond lowest order. In view of this delicate balancing between divergences, the check of our analytic expressions against the numerical results of Stecki and Dudowicz is most welcome.

The basic reason why C increases without bounds when the average height moves away from the interface is the fact that the bulk phases in our model are incompressible. The incompressibility causes $H \to 0$ when $z_1, z_2 \to \pm\infty$, and C, inversely related to H, must diverge. Allowing for density fluctuations, however small, in the bulk phases, will force C to reach a finite bulk value when $z_1, z_2 \to \pm\infty$. That this is so for the genuine lattice gas (not the solid-on-solid version) is indicated by the computations of Dudowicz and Stecki (1985). To perform the same asymptotic analysis for the genuine lattice gas as we present here for the solid-on-solid version seems, unfortunately, not feasible.

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