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LETTER TO THE EDITOR

Fluctuations of interfaces and anisotropy

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Abstract. The mean square vertical displacement W^2 is considered for $(1+1)$ -dimensional interfaces of the SOS type which make an angle θ with respect to the horizontal axis. It is proved that W^2 per unit horizontal length is proportional to the inverse of $\beta\gamma(\theta) + \beta\gamma''(\theta)$, where β is the inverse temperature, $\gamma(\theta)$ is the surface tension of the interface at angle θ and $\gamma''(\theta)$ is the second derivative of γ with respect to its argument. This result establishes, on a microscopic basis, the validity of the corresponding formula proposed by Akutsu and Akutsu using thermodynamical arguments.

The microscopic description of interfaces has been a subject of considerable activity during the last 30 years. In particular, several works have been devoted to the study of interface fluctuations.

There are essentially two kinds of approach to describe the properties of interfaces.

The first one, the so-called local free energy approach, rests upon a concentration profile $\rho(z)$ (where z is the vertical direction) (Widom 1972, Rowlinson and Widom 1982). It leads to a density profile width independent of the system size. However Abraham and Reed (1976) have shown that this prediction is not in agreement with the result obtained for the two-dimensional Ising ferromagnet.

The second approach, based on capillary wave theory, introduced by Buff *et al* (1965) and Weeks (1977), gives a precise prediction for the mean square displacement of the interface in the vertical direction. Let W^2 denote this quantity. In its original form it was proposed that W^2 behaves like

$$W^2/L \sim 1/\beta\gamma \quad (1)$$

where γ is the surface tension characterising the interface, β is the inverse temperature and L is the size of the interface.

In an interesting piece of work, Abraham (1981) (see also Abraham and Reed 1977) pointed out that an exact calculation within the two-dimensional Ising model leads to a different result:

$$W^2/L \sim 1/\sinh \beta\gamma. \quad (2)$$

The agreement between this result and capillary wave theory has been recovered by Fisher *et al* (1982). They realised that (1) only holds for isotropic media and derived heuristically the following correction for an interface parallel to the horizontal axis in the mean, taking into account anisotropic effects:

$$W^2/L \sim 1/\beta(\gamma(0) + \gamma''(0)) \quad (3)$$

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where $\gamma(\theta)$ is the surface tension for an interface with average angle θ with respect to the horizontal axis, $\gamma''(0)$ denotes the second derivative of γ with respect to θ considered at $\theta = 0$.

Rather recently, a generalisation of this formula has been proposed by Akutsu and Akutsu (1986). On a thermodynamical basis they proposed the following equation:

$$W_\theta^2/L \sim 1/\beta(\gamma(\theta) + \gamma''(\theta)) \quad (4)$$

for an interface which makes an angle θ in the mean with the horizontal axis. These authors showed by an explicit calculation for one microscopic model the validity of their formula (4), and use it within the two-dimensional Ising ferromagnet where $\gamma(\theta)$ is explicitly known (Abraham and Reed 1977).

However, at least to our knowledge, a rigorous general proof of this result is still lacking. This is precisely the aim of this letter. Using statistical mechanical considerations, we establish hereafter the validity of equation (4) for (1+1)-dimensional models of the solid-on-solid type.

Let us first define the class of models we consider by introducing a Hamiltonian which characterises a wandering interface: $H(h_0, h_1, \dots, h_L)$, where h_i denotes the height of the interface at point i (there are therefore no overhangs). Typical examples are given by (a) the continuous sos model:

$$H(h_0, h_1, \dots, h_L) = -J \sum_0^{L-1} |h_{i+1} - h_i| \quad \text{where } h_i \in \mathbb{R}, J > 0$$

(b) the restricted sos model:

$$H(h_0, h_1, \dots, h_L) = -J \sum_0^{L-1} |h_{i+1} - h_i| \quad \text{where } h_i \in \{0, +1, -1\}, J > 0$$

and (c) the continuous Gaussian model:

$$H(h_0, h_1, \dots, h_L) = -J \sum_0^{L-1} (h_{i+1} - h_i)^2 \quad \text{where } h_i \in \mathbb{R}, J > 0.$$

More generally, we shall consider hereafter the class of Hamiltonians

$$H(h_0, h_1, \dots, h_L) = - \sum_0^{L-1} P(h_{i+1} - h_i)$$

where $P(x)$ is an even polynomial bounded from below. For this class of models, let us now introduce the surface tension at angle θ : $\gamma(\theta)$. Its statistical mechanical definition is given by

$$\frac{\beta\gamma(\theta)}{\cos \theta} = - \lim_{L \rightarrow \infty} \frac{1}{L} \log \int_{-\infty}^{+\infty} dh_0 \dots \int_{-\infty}^{+\infty} dh_L \times \exp[-\beta H(h_0, h_1, \dots, h_L)] \delta(h_0) \delta(h_L - L \tan \theta) \quad (5)$$

where δ denotes the Dirac measure.

To compute the fluctuations of the interface along the vertical axis, one has to evaluate the asymptotic behaviour of ($0 < \alpha < 1$, $\alpha \cdot L \in \mathbb{N}$)

$$(1/L) \langle (\phi_{\alpha L})^2 \rangle$$

where ϕ_i is the random variable associated to the difference between the interface and the straight line which makes an angle θ with the horizontal axis (see figure 1), i.e.

$$\phi_i = h_i - i \tan \theta.$$

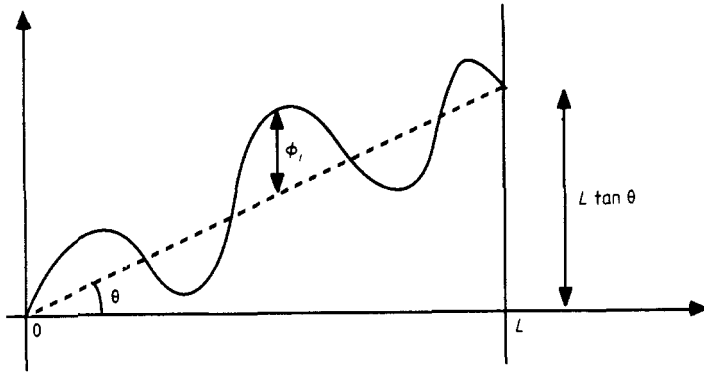


Figure 1. Vertical displacement of interface with respect to the straight line $y = x \tan \theta$.

The mean value $\langle \phi_i \rangle$ has to be computed with respect to the probability measure induced by (5). One therefore has to analyse the following quantity:

$$\begin{aligned} \langle \phi_i^2 \rangle &= \left[\int_{-\infty}^{+\infty} d\phi_0 \dots \int_{-\infty}^{+\infty} d\phi_L \exp\left(-\beta \sum P(\phi_{i+1} - \phi_i + \tan \theta)\right) \delta(\phi_0) \delta(\phi_L) \right]^{-1} \\ &\quad \times \int_{-\infty}^{+\infty} d\phi_0 \dots \int_{-\infty}^{+\infty} d\phi_L \phi_i^2 \exp\left(-\beta \sum P(\phi_{i+1} - \phi_i + \tan \theta)\right) \delta(\phi_0) \delta(\phi_L). \end{aligned}$$

This is realised in the following theorem.

Theorem. For $(1+1)$ -dimensional interfaces (h_0, h_1, \dots, h_L) with probability density proportional to

$$\exp\left(-\beta \sum P(|h_{i+1} - h_i|)\right)$$

where $P(x)$ is an even polynomial bounded from below, the fluctuations of the interface along the vertical direction behave asymptotically as

$$\lim_{L \rightarrow \infty} \left\langle \left(\frac{\phi_{\alpha L}}{[\alpha(1-\alpha)L]^{1/2}} \right)^2 \right\rangle = \frac{1}{\beta(\gamma(\theta) + \gamma''(\theta))} \frac{1}{\cos^3 \theta} \tag{6}$$

for an inclination of θ in the mean and for any $0 < \alpha < 1$.

Proof. The proof proceeds in two steps. We shall first show that, as $L \rightarrow \infty$, we have

$$\frac{1}{\alpha(1-\alpha)L} \langle (\phi_{\alpha L})^2 \rangle \rightarrow w_\theta^2 = \int_{-\infty}^{+\infty} x^2 q_\theta(x) dx \tag{7}$$

where

$$q_\theta(x) = \exp[-\beta P(x + \tan \theta) + c_\theta x] dx \left(\int_{-\infty}^{+\infty} \exp[-\beta P(x + \tan \theta) + c_\theta x] dx \right)^{-1}$$

and c_θ is the solution of

$$\int_{-\infty}^{+\infty} x q_\theta(x) dx = 0.$$

The second step will then be to show that

$$w_\theta^2 = \frac{1}{\beta(\gamma(\theta) + \gamma''(\theta))} \frac{1}{\cos^3 \theta}. \tag{8}$$

First step of the proof. Since

$$\phi_i = \sum_{j=1}^i (\phi_j - \phi_{j-1}) + \phi_0 \equiv \sum_{j=0}^i X_j$$

with $X_0 = \phi_0$, we shall have

$$\frac{1}{L} \langle (\phi_{\alpha L})^2 \rangle = \frac{1}{L} \sum_{k=1}^{\alpha L} \sum_{l=1}^{\alpha L} \langle X_k X_l \rangle \tag{9}$$

where

$$\begin{aligned} \langle X_k X_l \rangle &= \left[\int_{-\infty}^{+\infty} dx_1 \dots \int_{-\infty}^{+\infty} dx_L \exp\left(-\beta \sum P(x_j + \tan \theta)\right) \delta\left(\sum x_j\right) \right]^{-1} \\ &\quad \times \int_{-\infty}^{+\infty} dx_1 \dots \int_{-\infty}^{+\infty} dx_L x_k x_l \exp\left(-\beta \sum P(x_j + \tan \theta)\right) \delta\left(\sum x_j\right) \end{aligned} \tag{10}$$

or equivalently for any real c

$$\begin{aligned} \langle X_k X_l \rangle &= \left[\int_{-\infty}^{+\infty} dx_1 \dots \int_{-\infty}^{+\infty} dx_L \delta\left(\sum x_j\right) \exp\left(\sum [-\beta P(x_j + \tan \theta) + cx_j]\right) \right]^{-1} \\ &\quad \times \int_{-\infty}^{+\infty} dx_1 \dots \int_{-\infty}^{+\infty} dx_L x_k x_l \delta\left(\sum x_j\right) \exp\left(\sum [-\beta P(x_j + \tan \theta) + cx_j]\right). \end{aligned}$$

In the following we shall show that

$$\frac{1}{\alpha(1-\alpha)L} \langle (\phi_{\alpha L})^2 \rangle = \int_{-\infty}^{+\infty} x^2 q_\theta(x) dx + O\left(\frac{1}{L^{1/2}}\right)$$

which establishes the validity of (7). Our method is inspired from one technique of the proof used in De Coninck and Dunlop (1987) and De Coninck *et al* (1987). Let us first rewrite (10) in a more suitable form:

$$\begin{aligned} \langle X_k X_l \rangle &= \left(\int_{-\infty}^{+\infty} dx_k \int_{-\infty}^{+\infty} dx_l q_\theta(x_k) q_\theta(x_l) f_{\Sigma_{L-2}}(x_k + x_l) \right)^{-1} \\ &\quad \times \int_{-\infty}^{+\infty} dx_k \int_{-\infty}^{+\infty} dx_l x_k x_l q_\theta(x_k) q_\theta(x_l) f_{\Sigma_{L-2}}(x_k + x_l) \end{aligned}$$

where

$$f_{\Sigma_{L-2}}(x) = \int_{-\infty}^{+\infty} \prod_{\substack{j=1 \\ j \neq k, l}}^L dx_j q_\theta(x_j) \delta\left(\sum_{j \neq k, l} x_j + x\right).$$

Using a local form of the central limit theorem (the so-called Edgeworth expansion for a density) (Feller 1971), we get uniformly in x :

$$\left| f_{\Sigma_{L-2}}(x) - \eta(x) - \eta(x) \sum_{k=3}^4 L^{1-k/2} P_k(x) \right| = O\left(\frac{1}{L^{3/2}}\right)$$

where

$$P_3(x) = \frac{\mu_3}{6\sigma^3} (x^3 - 3x)$$

$$P_4(x) = \frac{\mu_3^2}{72\sigma^6} (x^3 - 3x) + \frac{\mu_4 - 3\sigma^4}{24\sigma^4} (x^4 - 6x^2 + 3)$$

$$\mu_k = \int_{-\infty}^{+\infty} x^k q_\theta(x) dx \quad \eta(x) = \frac{1}{\sqrt{2\pi}} \exp(-\frac{1}{2}x^2) \quad \sigma^2 = \mu_2$$

provided that the fifth moment indeed exists (this is guaranteed by our hypotheses on P). Since we have for densities of probability:

$$f_{aX+b}(x) - \frac{1}{a} f_X\left(\frac{x-b}{a}\right)$$

for any reals $a > 0$ and b , we get

$$\sigma\sqrt{L} f_{\Sigma_L}(x) = \eta\left(\frac{x}{\sigma\sqrt{L}}\right) \left(1 + \frac{\mu_4 - 3\sigma^4 - 4\mu_3x}{8L\sigma^4}\right) + O\left(\frac{1}{L^{3/2}}\right).$$

Using this result, we obtain for $\langle X_k X_l \rangle$:

$$\begin{aligned} & \left[\int_{-\infty}^{+\infty} dx_k dx_l q_\theta(x_k) q_\theta(x_l) \left(1 + \frac{A+B(x_k+x_l)}{L}\right) \exp\left(-\frac{(x_k+x_l)^2}{2L\sigma^2}\right) + O\left(\frac{1}{L^{3/2}}\right) \right]^{-1} \\ & \times \int_{-\infty}^{+\infty} dx_k dx_l x_k x_l q_\theta(x_k) q_\theta(x_l) \left(1 + \frac{A+B(x_k+x_l)}{L}\right) \\ & \times \exp\left(-\frac{(x_k+x_l)^2}{2L\sigma^2}\right) + O\left(\frac{1}{L^{3/2}}\right) \end{aligned}$$

where A and B are real constants. It remains to use the following inequality:

$$1 - \frac{1}{2}y^2 \leq \exp(-\frac{1}{2}y^2) \leq 1 - \frac{1}{2}y^2 + \frac{1}{8}y^4$$

which holds for any real y , to obtain

$$\langle X_k X_l \rangle = -\frac{\sigma^2}{L} + O\left(\frac{1}{L^{3/2}}\right) \quad \text{for } k \neq l. \tag{11}$$

On the other hand, for $k = l$, we have

$$\begin{aligned} \langle X_k^2 \rangle &= \left[\int_{-\infty}^{+\infty} dx q_\theta(x) \left(1 + \frac{A+Bx}{L}\right) \exp\left(-\frac{x^2}{2L\sigma^2}\right) + O\left(\frac{1}{L^{3/2}}\right) \right]^{-1} \\ & \times \int_{-\infty}^{+\infty} dx x^2 q_\theta(x) \left(1 + \frac{A+Bx}{L}\right) \exp\left(-\frac{x^2}{2L\sigma^2}\right) + O\left(\frac{1}{L^{3/2}}\right) \end{aligned}$$

which leads to

$$\langle X_k^2 \rangle = \sigma^2 + O\left(\frac{1}{L}\right). \tag{12}$$

Combining (11) and (12) we get

$$\frac{1}{L} \sum_{k=1}^{\alpha L} \sum_{l=1}^{\alpha L} \langle X_k X_l \rangle = \alpha(1-\alpha)\sigma^2 + O\left(\frac{1}{\sqrt{L}}\right)$$

which establishes the validity of (7).

Second step of the proof. It has been proved in De Coninck and Dunlop (1987) that

$$\beta\gamma(\theta) = -\cos \theta \log z(\theta)$$

where

$$z(\theta) = \int_{-\infty}^{+\infty} \exp[-\beta P(x + \tan \theta) + c_\theta x] dx$$

and c_θ has to be defined as the solution of

$$\int_{-\infty}^{+\infty} x q_\theta(x) dx = 0$$

or, in other words, c_θ must verify

$$\int_{-\infty}^{+\infty} x \exp[-\beta P(x) + c_\theta x] dx = \tan \theta \int_{-\infty}^{+\infty} \exp[-\beta P(x) + c_\theta x] dx.$$

A simple derivation of $z(\theta)$ with respect to θ leads to the identity

$$z'(\theta) = -c_\theta(1 + \tan^2 \theta)z(\theta)$$

from which we easily get

$$\beta(\gamma(\theta) + \gamma''(\theta)) = c'_\theta / \cos \theta. \quad (13)$$

Since

$$\begin{aligned} w_\theta^2 &= \int_{-\infty}^{+\infty} x^2 \exp[-\beta P(x + \tan \theta) + c_\theta x] dx \left(\int_{-\infty}^{+\infty} \exp[-\beta P(x + \tan \theta) + c_\theta x] dx \right)^{-1} \\ &= \int_{-\infty}^{+\infty} x^2 \exp[-\beta P(x) + c_\theta x] dx \left(\int_{-\infty}^{+\infty} \exp[-\beta P(x) + c_\theta x] dx \right)^{-1} - \tan^2 \theta \end{aligned}$$

it is straightforward to show that

$$w_\theta^2 = (1 + \tan^2 \theta) / c'_\theta. \quad (14)$$

It remains to compare (13) with (14) to achieve the proof of the theorem.

Let us also stress that the validity of our theorem can be extended to more general models. The expression (6) holds whenever the probability density $q_\theta(x)$ admits moments up to sixth order. Using appropriate central limit theorems in a local form (Petrov 1975), it can be shown that discrete probability distributions may also be considered, like for instance the one which appears in the discrete SOS model.

As a typical example of the importance of the anisotropic effect, we give hereafter $\beta\gamma(0)$ and $\beta(\gamma(0) + \gamma''(0))$ for the Gaussian continuous model. We have

$$\beta\gamma(0) = \frac{1}{2} \log(\beta J / \pi)$$

$$\beta(\gamma(0) + \gamma''(0)) = 2\beta J.$$

This result clearly shows, once more, the importance of anisotropy within interface phenomena. It should also be noticed that this last expression is in perfect agreement with the vanishing of the width of the interface at $T = 0$.

As a final remark, we would like to point out that our formula (6) is slightly different from the result of Akutsu and Akutsu (1986). The difference has to be found in the factor $1/\cos^3 \theta$ which disappears if we consider the fluctuations of the interface perpendicularly to the straight line $i \tan \theta$ per unit length of the interface.

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Note added. After finishing this work we became aware of one result of Abraham (1987) establishing the validity of relation (4) within the two-dimensional Ising model.

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