Width of Rough Interfaces
on Asymmetric Lattices

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Abstract

I present a calculation of the interfacial width within the capillary wave (Gaussian) approximation. The calculation is done on rectangular lattices of size $L_1$ times $L_2$, with periodic boundary conditions.
1 Introduction

The two-dimensional interface separating the phases of a 3D binary system can undergo a roughening transition [1]. Below the roughening temperature, the interface has a finite width in the infinite volume limit. The rough phase, however, is characterized by strong fluctuations of the interface position variables, and the interface width diverges when the area of the surface goes to infinity. Properties of the roughening transition have been investigated in a variety of studies, see e.g. [2] and references therein. It is generally believed, and has been confirmed in a number of numerical studies [3], that the infrared (large distance) properties of a rough interface can be described by massless Gaussian modes. This concept was introduced by Buff et al. [4] and is usually referred to as the capillary wave model (CWM). The CWM allows to make predictions, e.g., about the finite size effects of various interface properties [3, 9]. Quite some attention has been devoted to asymmetric interfaces, where the two extensions $L_1$ and $L_2$ of a rectangular interface do not necessarily coincide [6, 7, 8, 10]. In [8, 9, 10] an extended (non-Gaussian) CWM was employed with an action proportional to the interface surface. The interface shape dependence was investigated in a field theoretic setting in [12].

In this article, I present a calculation of the interface width on asymmetric rectangular lattices, within the CWM. Related calculations with a continuum cutoff were done in a gauge theory setting in [11]. Interestingly, the lattice result obtained in the present paper points the way to a significant simplification of the continuum result presented in [11].

2 The Lattice Capillary Wave Model

Let the interface (without overhangs) be described by a “height” function $\varphi_x$, where $x$ is a site of a two-dimensional grid with side lengths $L_1$ and $L_2$. We choose units such that the lattice spacing is dimensionless and assume that it is one for both lattice directions. We employ periodic boundary conditions.

Within the capillary wave approximation for the fluctuations of the height variables, expectation values are defined by

$$\langle O \rangle = \lim_{m \to 0} \frac{\int \prod_x d\varphi_x e^{-H_0(\varphi)} O(\varphi)}{\int \prod_x d\varphi_x e^{-H_0(\varphi)}},$$

where $O$ is any physical quantity of interest.
with the Hamiltonian (energy functional)

\[ H_0(\varphi) = \frac{1}{2\beta} \sum_{x,y} (\varphi_x - \varphi_y)^2 + \frac{m_1^2}{2} \sum_x \varphi_x^2. \]

The first term is a sum over all nearest neighbour bonds in the lattice. We define the interface width (or surface thickness) by

\[ W^2 = \frac{1}{L_1 L_2} \sum_x \langle (\varphi_x - \varphi_{x_0})^2 \rangle, \]

where \( x_0 \) is an arbitrary site of the lattice. The interfacial width can also be written as

\[ W^2 = 2 \langle (\varphi_{x_0} - \phi)^2 \rangle, \]

where \( \phi = \sum_x \varphi_x \) is the average interface position. In the following section we will show that

\[ \frac{W^2}{2\beta} = K + \frac{\ln L_1 L_2}{4\pi} - \frac{1}{\pi} \ln \left( u^{1/4} \eta(iu) \right) + \frac{1}{L_1 L_2} Z(u) + O \left( \left( L_1 L_2 \right)^{-2} \right). \] (1)

\( \eta \) is the Dedekind function. We will compute explicit expressions for the constant \( K \) and the function \( Z(u) \) that depends on the asymmetry-parameter \( u \equiv \frac{L_2}{L_1} \).

### 3 Calculation of \( W^2 \)

By means of discrete Fourier transformation \( W^2 \) can easily shown to be

\[ W^2 = \frac{2\beta}{L_1 L_2} \sum_{p \neq 0} \frac{1}{p_1^2 + p_2^2}. \]

The lattice momenta are defined by \( p_i = \frac{2\pi}{L_i} n_i \), with \( n_i = 0, \ldots, L_i - 1 \), and \( p_i^2 = 4 \sin^2 \frac{\theta}{2} \). Let us rewrite the sum excluding \( p = (p_1, p_2) = 0 \) in the following way:

\[ \sum f(n_1, n_2) = \sum_{n_2=1}^{L_2-1} f(0, n_2) + \sum_{n_1=1}^{L_1-1} \sum_{n_2=0}^{L_2-1} f(n_1, n_2). \]
Employing the identity
\[
\frac{1}{\sinh^2(x/2) + \sin^2(\omega/2)} = \frac{2}{\sinh x} \sum_{n=-\infty}^{\infty} e^{-x|n|} e^{-i\omega n},
\]
we can perform a first summation:
\[
\sum_{n_2=0}^{L_2-1} \frac{1}{\sin^2 \left( \frac{\pi n_1}{L_1} \right) + \sin^2 \left( \frac{\pi n_2}{L_2} \right)} = \frac{2L_2}{\sinh X_{n_1}} \left( 1 + 2 e^{-L_2 X_{n_1}} \right) \cdot (2)
\]
The quantity \(X_{n_1}\) is defined by
\[
\sinh \left( \frac{X_{n_1}}{2} \right) = \sin \left( \frac{\pi n_1}{L_1} \right).
\]
Performing a suitable limit, one can use eq. (2) to show that
\[
\sum_{n_2=1}^{L_2-1} \frac{1}{\sin^2 \left( \frac{\pi n_2}{L_2} \right)} = \frac{1}{3} (L_2^2 - 1) .
\]
Putting things together, we find
\[
\frac{W^2}{2\beta} = \frac{1}{12} \frac{L_2^2 - 1}{L_1 L_2} + \frac{1}{2L_1} \sum_{n_1=1}^{L_1-1} \frac{1}{\sinh X_{n_1}} \left( 1 + 2 e^{-L_2 X_{n_1}} \right) \cdot \frac{L_1}{1 - e^{-L_2 X_{n_1}}} .
\]
We shall first study the sum
\[
S = \frac{1}{2L_1} \sum_{n_1=1}^{L_1-1} \frac{1}{\sinh X_{n_1}} .
\]
Note that
\[
\sinh X_{n_1} = 2 \sinh \left( \frac{X_{n_1}}{2} \right) \cosh \left( \frac{X_{n_1}}{2} \right) = 2 \sin \left( \frac{\pi n_1}{L_1} \right) \sqrt{1 + \sin^2 \left( \frac{\pi n_1}{L_1} \right)} .
\]
Exploiting that \(\sin (\pi n_1/L_1) = \sin (\pi (L_1 - n_1)/L_1)\) and assuming that \(L_1 \equiv 2M_1\) is even, we obtain
\[
S = 2 \sum_{n_1=1}^{M_1-1} g(X_{n_1}) + g(M_1), \quad (3)
\]
with \( g(x_{n_1}) = (2L_1 \sinh(X_{n_1}))^{-1} \). \( S \) can then be represented as \( S = S_1 + S_2 \), where

\[
S_1 = \sum_{n_1=1}^{M_1-1} \left( \frac{1}{2L_1 \sin \left( \frac{\pi n_1}{L_1} \right)} \sqrt{1 + \sin^2 \left( \frac{\pi n_1}{L_1} \right)} - \frac{1}{2\pi n_1} \right) + \frac{1}{4\sqrt{2L_1}} ,
\]

and

\[
S_2 = \frac{1}{2\pi} \sum_{n_1=1}^{M_1-1} \frac{1}{n_1} .
\]

The sum \( S_1 \) can be evaluated with the help of the Euler-Mc-Laurin summation formula. One finds

\[
S_1 = \frac{1}{2\pi} \left( \frac{3}{2} \ln 2 - \ln \pi + \frac{1}{L_1} + \left( \frac{1}{3} + \frac{\pi^2}{36} \right) \frac{1}{L_1^2} \right) + O \left( L_1^{-4} \right) .
\]

\( S_2 \) can also be summed:

\[
S_2 = \frac{1}{2\pi} \left( C + \psi(M_1) \right) ,
\]

where \( C = 0.5772... \) denotes Euler’s constant, and \( \psi \) is the Digamma function. We expand

\[
S_2 = \frac{1}{2\pi} \left( \ln 2 + \ln L_1 + C - \frac{1}{L_1} - \frac{1}{3L_1^2} \right) + O \left( L_1^{-4} \right) .
\]

\( S \) thus combines to

\[
S = \frac{1}{2\pi} \left( C + \frac{1}{2} \ln 2 - \ln \pi + \ln L_1 \right) + \frac{\pi}{72L_1^2} + O \left( L_1^{-4} \right) .
\]

Our next task is to study

\[
T = \frac{1}{L_1} \sum_{n_1=1}^{L_1-1} \frac{1}{\sinh(X_{n_1})} \frac{e^{-L_2X_{n_1}}}{1 - e^{-L_2X_{n_1}}} .
\]

As for eq. (3), we use the symmetry of the “integrand” to write

\[
T = \sum_{n_1=1}^{M_1-1} h(X_{n_1}) + h(X_{M_1}) , \tag{4}
\]
with
\[ h(X_{n_1}) = \frac{1}{L_1 \sinh(X_{n_1})} \frac{e^{-L_2 X_{n_1}}}{1 - e^{-L_2 X_{n_1}}} . \]

Recall that \( M_1 = L_1/2 \), and that we have assumed that \( L_1 \) is even. We are interested in the limit \( L_1 \to \infty \), with the ratio \( u = L_2/L_1 \) kept fixed. One first observes that the contribution \( h(X_{M_1}) \) vanishes exponentially fast in this limit, namely like \( \exp(-2 \arcsinh(1) u L_1) \). For large \( L_1 \), we expand
\[ h(X_{n_1}) = \frac{1}{\pi} \frac{q^{n_1}}{n_1 (1 - q^{n_1})} (1 + A(n_1, L_1, u)) , \]
where
\[ q \equiv \exp(-2\pi u) . \]

We obtain
\[ A(n_1, L_1, u) = \frac{1}{L_1^2} \frac{\pi^2 n_1^2}{3} \left( \frac{2\pi n_1 u}{1 - q^{n_1}} - 1 \right) + O\left(L_1^{-4}\right) . \]

Extending the sum in eq. (4) to the range 1 to infinity introduces only errors that are exponentially small in \( L_1 \). We thus find
\[ T = \frac{1}{\pi} \sum_{n=1}^{\infty} \frac{q^n}{n (1 - q^n)} + \frac{1}{L_1^3} \left( \frac{2\pi^2}{3} u \sum_{n=1}^{\infty} \frac{n^2 q^n}{(1 - q^n)^2} - \frac{\pi}{3} \sum_{n=1}^{\infty} \frac{n q^n}{1 - q^n} \right) + O\left(L_1^{-4}\right) . \]

Let us define
\[ F(u) = \sum_{n=1}^{\infty} \frac{q^n}{n (1 - q^n)} , \]
\[ G(u) = \sum_{n=1}^{\infty} \frac{n^2 q^n}{(1 - q^n)^2} , \]
\[ H(u) = \sum_{n=1}^{\infty} \frac{n q^n}{1 - q^n} . \]

Noting that \( \ln L_1 = \frac{1}{2} \ln (L_1 L_2) - \frac{1}{2} \ln u \), and putting everything together, we obtain
\[ \frac{W^2}{2\beta} = K + \frac{\ln L_1 L_2}{4\pi} - \frac{1}{\pi} \ln \left(u^{1/4} \eta(iu)\right) + \frac{1}{L_1 L_2} Z(u) + O\left((L_1 L_2)^{-2}\right) . \] (5)

The constant \( K \) is given by
\[ K = \frac{1}{2\pi} \left(C + \frac{1}{2} \ln 2 - \ln \pi \right) . \]
Furthermore, we have used that $F(u) = G_1(q)$, where

$$G_p(x) = \sum_{n=1}^{\infty} \frac{x^n}{n^p (1 - x^n)}$$

is Lambert’s series \textsuperscript{13}. For $p = 1$, it is related to Dedekind’s $\eta$-function,

$$G_1 \left( e^{-2\pi u} \right) = -\frac{\pi u}{12} - \ln \eta(iu) ,$$

with

$$\eta(iu) = q^{1/24} \prod_{n=1}^{\infty} (1 - q^n).$$

The symmetry of the interface width under exchange of $L_1$ and $L_2$ should be reflected in an invariance under the transformation $u \to 1/u$. It is well known that $u^{1/4} \eta(iu)$ is invariant under this transformation.

The part proportional to $(L_1 L_2)^{-1}$ is given by

$$Z(u) = \frac{\pi}{72} u - \frac{1}{12} + \frac{2\pi^2}{3} u^2 G(u) - \frac{\pi}{3} u H(u) .$$

We would like to demonstrate that this expression is invariant under $u \to 1/u$. To this end we first observe that

$$H(u) = \frac{1}{24} \left( 1 - E_2(iu) \right) ,$$

with $E_2$ being the first Eisenstein series. It obeys the functional relation

$$E_2(iu) = -u^{-2} E_2(iu^{-1}) + \frac{6}{\pi} u^{-1} . \quad (6)$$

The crucial step is now to recognize that $G$ can be written as

$$G = q \frac{d}{dq} H = -\frac{1}{48\pi} \frac{d}{du} E_2(iu) .$$

We then have

$$Z(u) = \frac{\pi}{72} \left( u E_2(iu) + u^2 \frac{d}{du} E_2(iu) \right) - \frac{1}{12} . \quad (7)$$

Differentiating eq. (3) with respect to $u$ yields the behaviour of $\frac{d}{du} E_2(iu)$ under $u \to 1/u$. Using this and eq. (3), it is easy to demonstrate the invariance of the right hand side of eq. (7).
We remark that it would be easy (though technical) to extend eq. (5) to higher orders in \((L_1 L_2)^{-1}\).

A comparison with eq. (A.4) of ref. [11] leads to an interesting observation. For the interface thickness on the continuum torus, regularized by a point splitting procedure, the authors obtain (I adapted their notation to the present setting)

\[
2\pi \sigma W^2 = \ln \left( L_1 \sqrt{1 + u^2} / 2 \varepsilon \right) + \frac{1}{2u} \arctan u + \frac{u}{2} \arctan \frac{1}{u} - \frac{3}{2} - \frac{\pi u}{12} \\
- \sum_{k=1}^{\infty} \frac{(1+u^2)E_{2k}(iu)}{2k u (2k+2)!} \left( (1 + u^2) \pi^2 \right)^k B'_k \sin \left( (2k + 2) \arctan u \right).
\]  

(8)

Here, \(E_{2k}(iu) = 1 + (-1)^k 4k \sum_{n=1}^{\infty} \frac{n^{2k-1} q^n}{1 - q^n}\) is the \(k\)'th Eisenstein series, and \(B'_k\) are Bernoulli numbers, defined through

\[
\frac{e^z}{e^z - 1} = 1 - \frac{z}{2} - \sum_{k=1}^{\infty} (-1)^k \frac{B'_k}{(2k)!} z^{2k}.
\]  

(9)

Comparing eq. (8) with the infinite area limit of eq. (5), and identifying \(\sigma \equiv 1/(2\beta)\), one is led to conjecture the identity

\[
\frac{1}{2} \ln(1 + u^2) + g(u) = -2 \ln \eta(iu) - C,
\]  

(10)

with

\[
g(u) = \frac{1}{2u} \arctan u + \frac{u}{2} \arctan \frac{1}{u} - \frac{3}{2} - \frac{\pi u}{12} \\
- \sum_{k=1}^{\infty} \frac{(1+u^2)E_{2k}(iu)}{2k u (2k+2)!} \left( (1 + u^2) \pi^2 \right)^k B'_k \sin \left( (2k + 2) \arctan u \right).
\]  

(11)

Eq. (10) turns out to be true, with \(C = -\ln(\pi)\), thus leading to an enormous simplification of the result of [11]. I will only give a sketch of the proof. One uses that

\[
\sin((2k + 2) \arctan(u)) = (1 + u^2)^{-k-1} \text{Im} \left( 1 + iu \right)^{2k+2}.
\]

One then meets the following two expressions to be evaluated:

\[
Y = \frac{1}{\pi^2 u} \text{Im} \sum_{k=1}^{\infty} \frac{B'_k}{2(2k+2)!} (\pi(1 + iu))^{2k+2}
\]
and
\[ V = -\frac{2}{\pi^2 u} \text{Im} \sum_{n=1}^{\infty} \frac{q^n}{n^3(1-q^n)} \sum_{k=1}^{\infty} \frac{(-1)^k}{(2k+2)!} (n\pi(1+iu))^{2k+2} \]

The latter expression can be evaluated by first doing the \(k\)-sum (yielding a \(\cos\) minus the two leading terms) and then extracting the imaginary part. One then again recognizes Lambert’s series with \(p = 1\), and ends with
\[ V = -\frac{\pi u}{6} - 2 \ln \eta(iu). \]

For the study of \(Y\), formula (A.6) of [11] is very helpful:
\[ \sum_{k=1}^{\infty} \frac{(-1)^k}{2k(2k+2)!} z^{2k+2} = \sum_{m=1}^{\infty} \frac{e^{-mz} - 1}{m^3} + \frac{z^2}{2} \ln z + \frac{\pi^2}{6} z - \frac{3}{4} z^2 - \frac{z^3}{12}. \]

With \(z = \pi(-u+i)\), and noting that for \(u > 0\)
\[ \ln z = \ln \pi + \frac{1}{2} \ln(1+u^2) - i \arctan(1/u) + i\pi, \]
one arrives after some algebra at
\[ Y = -\ln \pi - \frac{1}{2} \ln(1+u^2) + \frac{1}{2u} \arctan \frac{1}{u} - \arctan \frac{1}{u} - \frac{3}{2} + \frac{\pi u}{4} - \frac{\pi}{4u}. \]

Combining things and noting that (for \(u > 0\)) \(\arctan u + \arctan \frac{1}{u} = \pi/2\), one arrives at eq. (10).

4 Concluding Remarks

The calculation presented in this paper is interesting at least for five reasons. First, it constitutes an illustrative example of analytical techniques that allow the exact evaluation of certain lattice sums. Second, the invariance under the exchange of the two lattice directions leads necessarily to the occurrence of modular forms and interesting relations between them. Third, the lattice result helped to simplify very much the continuum computation of ref. [11]. Fourth, interesting physical applications are possible, e.g., in the context of analytical and Monte Carlo calculations (cf. again [11]). Finally, the present approach gives the the \(1/\text{area}\) correction to the asymptotic behaviour of the interface thickness. This could be useful as a starting point to test the CWM “beyond the gaussian approximation” [9, 10] also for the interfacial width.
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