Capillary Wave Approach to Order-Order Fluid Interfaces in the 3D Three-State Potts Model

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Abstract

The physics of fluid interfaces between domains of different magnetization in the ordered phase of the 3D three-state Potts model is studied by means of a Monte Carlo simulation. It is shown that finite-size effects in the interface free energy are well described by the capillary wave model at two loop order, supporting the idea of the universality of this description of fluid interfaces in 3D statistical models.

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1 Introduction

It is well known that 3D spin systems on finite volumes show domain walls separating coexisting phases which behave as fluid interfaces between the critical and the roughening temperature. The finite-size effects in the free energy of a fluid interface are dominated by long-wavelength fluctuations and a correct physical description of the critical properties of the surface cannot neglect their contributions [1].

While below the roughening temperature, where the interfaces are almost rigid, a microscopical approach can be taken (see [2] and references therein), above it one is forced to assume an effective model describing the collective degrees of freedom of rough interfaces.

The capillary wave model (CWM) [3] in its simplest formulation, which we will follow, assumes an effective hamiltonian proportional to the area of the surface.

It has been recently shown [4] that rather strong finite-size effects, depending on the shape of the lattice, are well described in terms of the one-loop or gaussian approximation to the CWM: its predictions have been tested with high accuracy in the scaling region of the 3D Ising model. These one-loop corrections depend only on one adimensional parameter, namely on the asymmetry $z = R/T$ of the transverse sizes of an elongated lattice $R \times T \times L$ $(L \gg R,T)$ with periodic boundary conditions taken in all directions [5, 6, 4].

As it has been already pointed out [4], higher order corrections to the gaussian model can be taken into account to verify the CWM beyond the one-loop approximation. These higher order corrections can provide a more stringent test of the CWM model: in fact, while many different effective hamiltonians reduce to the gaussian form at one-loop level [7], they differ in the form of two- and higher-loop corrections. In this paper we apply the CWM in the two-loop approximation to the finite-size behavior of order-order rough interfaces in the 3D three-state Potts model.

The two-loop contributions do not depend only on the asymmetry parameter $z$ but also on an adimensional parameter proportional to the minimal area of the surface, namely $\sigma RT$, $\sigma$ being the (reduced) interface tension. An important consequence of this fact is that the well known finite-size behavior [8] of the energy splitting $E$ occurring between vacua on finite volumes, has no longer, at two-loop, the classical functional form

$$E_{cl}(R) \propto e^{-\sigma R^2}$$

not even for symmetric ($R = T$) lattices. This must be contrasted with what
happens at one–loop level, where, due to the scale–invariance of the one–loop contributions, one has to consider asymmetric lattices to find deviations from the classical functional form [4].

To verify the CWM we study the finite-size behavior of rough order–order interfaces of the 3D three-state Potts model by means of Monte Carlo numerical simulations.

This model is of great interest because of its well known connection with 4D $SU(3)$ pure Yang–Mills theory at finite temperature [9]. In fact one can assume an effective action of a 3D spin model with short–range, ferromagnetic interaction to describe the finite temperature deconfinement transition of QCD in the limit of infinite quark masses [10]. For this reason the Potts model has been extensively investigated and, in particular, the properties of order-order and order-disorder interfaces have been already studied [11, 12, 13], one of the main goals being the evaluation of the corresponding interface tensions.

In this paper we show that the knowledge of the functional form of the fluid interface free energy on finite volumes, including the capillary wave contributions, enables one to estimate the order-order interface tension with high precision. Moreover, the good agreement we find with the theoretical predictions of the CWM model at two–loop order strongly supports the idea of the universality of this description of rough interfaces in 3D statistical models.

The paper is structured as follows: in Sec. 2. we describe the CWM and its one–loop and two–loop approximations. In Sec. 3. we compare the results of MC simulations with the CWM predictions. Sec. 4 is devoted to some concluding remarks.

2 The capillary wave model

According to the CWM, the interface between two domains of different magnetization in the ordered phase of a 3D spin system, above the roughening temperature, is described by the partition function

$$Z_{cw} = \int [Dx] \exp \{-\sigma A[x]\},$$

where the single-valued function $x(r,t)$ describes the displacement from the equilibrium position of the interface, $\sigma$ is the reduced (order-order) interface tension and $A[x]$ is the area of the interface.
\[ A[x] = \int_0^R dr \int_0^T dt \sqrt{1 + \left( \frac{\partial x}{\partial r} \right)^2 + \left( \frac{\partial x}{\partial t} \right)^2} . \] (3)

It should be mentioned that (3) coincides with the Nambu-Goto string action in \( D = 3 \) in a particular gauge. Eq. (3) is not expected to be the exact action describing fluid interfaces but at least the dominant contribution\(^\dagger\): as we will show this is indeed the case.

To compare the predictions of the CWM with numerical results from Monte Carlo (MC) simulations, we have chosen 3D lattices of \( R \times T \times L \) sites, with \( L \gg R, T \), and periodic boundary conditions in each direction. This particular choice of the lattice shape allows one to consider only interfaces orthogonal to the elongated \((L)\) direction, the probability of having interfaces orthogonal to the other directions being negligible. The 2D field \( x(r, t) \) is therefore defined on the rectangle \((r, t) \in [0, R] \times [0, T] \) with opposite edges identified, i.e. on a torus.

The partition function (2) cannot be computed exactly, but it is possible to express it as an expansion in powers of the adimensional parameter \((\sigma RT)^{-1}\): the two–loop expansion of \( Z_{cw} \) can then be written as

\[
Z_{cw}(R,T) \propto e^{-\sigma RT} Z_q^{(1 \, \text{loop})} \left( \frac{R}{T} \right) \cdot Z_q^{(2 \, \text{loop})} (R, T) .
\] (4)

The one–loop contribution (namely the gaussian approximation), obtained retaining only the quadratic term in the expansion of (3), is nothing else than the exact partition function of a 2D conformal invariant free boson on a torus of modular parameter \( \tau = \frac{R}{T} \)[5, 6, 4]

\[
Z_q^{(1 \, \text{loop})} \left( \frac{R}{T} \right) = \sqrt{\frac{T}{R}} \left| \eta \left( \frac{R}{T} \right) \right|^{-2} ,
\] (5)

while the two–loop term can be calculated perturbatively expanding (3) at the next–to–leading order [15]

\[
Z_q^{(2 \, \text{loop})}(R, T) = 1 + \frac{1}{2\sigma RT} \left\{ \left[ \frac{\pi R}{6 T} E_2 \left( \frac{i R}{T} \right) \right]^2 - \frac{\pi R}{6 T} E_2 \left( \frac{i R}{T} \right) + \frac{3}{4} \right\}
+ O \left[ (\sigma RT)^{-2} \right] .
\] (6)

\(^\dagger\)The problems arising in the quantization of non–critical strings are known to disappear asymptotically at large distances [14].
The two functions $\eta$ and $E_2$ appearing above are respectively the Dedekind function and the second Eisenstein series:

$$\eta(\tau) = q^{1/24} \prod_{n=1}^{\infty} (1 - q^n), \quad q \equiv \exp(2\pi i \tau)$$

$$E_2(\tau) = 1 - 24 \sum_{n=1}^{\infty} \frac{n q^n}{1 - q^n}.$$ 

The three–state Potts model is defined by the partition function

$$Z = \sum_{\{\sigma_i\}} \exp \left\{ -\beta \sum_{i,\mu} \left[ 1 - \text{Re}(\sigma_i^\dagger \sigma_{i+\mu}) \right] \right\}$$  

(7)

where the variables $\sigma_i$ are defined on a three–dimensional hypercubic lattice and take the values

$$\sigma_i = \exp \left( \frac{2\pi in_i}{3} \right) \quad n_i = 0, 1, 2.$$  

(8)

In the thermodynamic limit the Potts model is known to undergo a (weak) first–order phase transition at $\beta_c = 0.36708(2)$ [16] and the roughening temperature can be estimate to be $\beta_r \sim 0.93$ [17]. For $\beta > \beta_c$ the $Z_3$ symmetry is spontaneously broken and the three ordered phases coexist, while at $\beta = \beta_c$ also the disordered phase coexists with the previous ones.

In the finite cylindrical geometry we are considering spontaneous symmetry breaking at low temperature cannot occur: the degeneracy of the ground state is removed, the energy of the symmetric, $Z_3$ invariant, ground state being separated by an energy splitting $E$ from the two degenerate mixed–symmetry states.

The energy splitting is due to tunneling between the phases and is directly linked to the free energy of the interface [8]. According to the CWM, for $\beta_r > \beta > \beta_c$, we assume [1, 3, 4], $R \geq T$,

$$E(R,T) = C e^{-\sigma RT} Z_q^{(1\ loop)} \left( \frac{R}{T} \right) \cdot Z_q^{(2\ loop)} (R,T)$$  

(9)

$$C = \frac{\delta}{Z_q^{(1\ loop)} (1)}$$
where $\delta$ is an unpredicted constant and a convenient normalization has been chosen.

We would like to stress that the two–loop contribution (6) does not depend only on the ratio $z = R/T$, like the one–loop term (5), but also on the minimal area $A_m = RT$. If we put $z = 1$, $A_m = R^2$, in (9) we obtain

$$E(R, R) = \delta e^{-\sigma R^2} \left\{ 1 + \frac{1}{2\sigma R^2} \left[ \left( \frac{\pi}{6} f \right)^2 - \frac{\pi}{6} f + \frac{3}{4} \right] \right\}, \quad (10)$$

where $f \equiv E_2(i)$. The classical formula [8]

$$E_{cl}(R) = \delta e^{-\sigma R^2} \quad (11)$$

can be recovered only neglecting the two–loop contribution.

The comparison between formula (9) and the values of $E$ extracted from MC simulations provides a simple and stringent way to verify the CWM predictions.

It should be noted that no new free parameters are introduced within this approach: the formulae (9) and (11) contain the same number of undetermined parameters, namely $\sigma$ and $\delta$.

### 3 Monte Carlo results

To extract the energy splitting $E$ from MC–generated ensembles we follow the procedure of [18]. Defining the time–slice magnetization

$$S_k \equiv \frac{1}{RT} \sum_{x_1=1}^{R} \sum_{x_2=1}^{T} \sigma(x_1, x_2, k), \quad (12)$$

we compute the correlation function

$$G(k) \equiv \langle S_0 S_k^* \rangle \quad (13)$$

where $k = 0, 1, \ldots, \frac{L}{2}$, and we extract the transfer matrix low energy levels from the asymptotic $k$–dependence of $G(k)$

$$G(k) \cdot Z = c_0 \left\{ \exp(-kE) + \exp[-(L-k)E] \right\} + c_1 \left\{ \exp(-kE') + \exp[-(L-k)E'] \right\} + \ldots \quad (14)$$

$$Z = 1 + 2e^{-LE} + \ldots \quad (15)$$
\[ Z \equiv \text{tr} \ e^{-LH} \] being the partition function (the next-to-leading energy level \( E' \) turns out to be non-negligible in our range of parameters).

Having so extracted the energy splitting \( E \) from the MC data for different values of the lattice sizes, we can compute the order-order interface tension \( \sigma \) and the constant \( \delta \) by fitting our data with the formula (9).

We have performed our simulations at \( \beta = 0.3680 \), the longest lattice size being fixed at \( L = 120 \), and the other sizes varying in the range \( 9 \leq T \leq 11, \ 10 \leq R \leq 36, \ (R \geq T) \). This value of \( \beta \) is enough inside the ordered phase to make highly suppressed the probability of formation of order-disorder interfaces [11] but presents a correlation length large enough to make the lattice artifacts negligible and to consider domain walls as fluid interfaces.

The fact that the disordered phase is substantially absent at this \( \beta \) can be seen from the histograms of the real part of the magnetization [19]

\[
\text{Re} M \equiv \text{Re} \left( \frac{1}{L} \sum_{k=1}^{L} S_k \right)
\]

as is shown, for example, in Fig. 1. The modulus of the magnetization at this \( \beta \) is about 0.44 – 0.50 for the lattice sizes we are considering: in this figure the projection on the real axis of the ordered phases are clearly visible while the peak centered at \( \text{Re} M = 0 \), which would signal the presence of the disordered phase, is absent.

Fig. 2 represents a typical distribution of the magnetization \( M \) for a sample of our MC-generated configurations. Most configurations consist of a single phase or of two phases separated by two interfaces (the minimum number compatible with periodic boundary conditions). The single-phase configurations are represented by the three clusters of points corresponding to the three degenerate vacua; the two-interface configurations form the straight lines joining these clusters. Three-interface configurations, which tend to fill uniformly the interior of the triangle, are clearly visible in Fig. 3: it corresponds to a \( T = 10, \ R = 20 \) lattice and to a larger probability of having tunneling events (i.e. interfaces), while these are much more suppressed for the lattice of Fig. 2 (\( T = R = 18 \)).

We have used a Swendsen-Wang cluster algorithm [20] to perform our MC simulations. To keep under control correlations in MC time and cross-correlations between the \( G(k) \) observables, we have systematically scattered our measurements avoiding the measurement of two different observables at the same MC time. We have made between \( 0.6 \cdot 10^6 \) and \( 1.8 \cdot 10^6 \) sweeps for each experiment, depending on the lattice size, obtaining about \( 10^3 \) data per
observable. However, the covariance matrix turns out to be different from the diagonal form, which one expects from a sample of statistical independent data. We have taken this fact into account by including the covariance matrix in the fitting procedure to formula (14) to extract the energy gap $E$: the results are reported in Tab. 1. The error on $E$ has been estimated with an ordinary jackknife procedure.

<table>
<thead>
<tr>
<th>$T$</th>
<th>$R$</th>
<th>$E$ (MC)</th>
<th>$\chi^2$</th>
<th>C.L.</th>
<th>$E$ (CWM)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>10</td>
<td>0.06399(51)</td>
<td>0.89</td>
<td>65%</td>
<td>0.06399</td>
</tr>
<tr>
<td>12</td>
<td>12</td>
<td>0.03924(54)</td>
<td>1.07</td>
<td>36%</td>
<td>0.03882</td>
</tr>
<tr>
<td>14</td>
<td>14</td>
<td>0.02201(54)</td>
<td>0.75</td>
<td>80%</td>
<td>0.02227</td>
</tr>
<tr>
<td>16</td>
<td>16</td>
<td>0.01234(32)</td>
<td>0.95</td>
<td>52%</td>
<td>0.01196</td>
</tr>
<tr>
<td>18</td>
<td>18</td>
<td>0.00508(71)</td>
<td>1.03</td>
<td>42%</td>
<td>0.00598</td>
</tr>
<tr>
<td>20</td>
<td>20</td>
<td>0.00305(68)</td>
<td>0.95</td>
<td>57%</td>
<td>0.00278</td>
</tr>
<tr>
<td>9</td>
<td>18</td>
<td>0.04108(73)</td>
<td>0.54</td>
<td>97%</td>
<td>0.04105</td>
</tr>
<tr>
<td>9</td>
<td>21</td>
<td>0.03467(96)</td>
<td>0.99</td>
<td>47%</td>
<td>0.03528</td>
</tr>
<tr>
<td>9</td>
<td>24</td>
<td>0.02933(11)</td>
<td>1.09</td>
<td>34%</td>
<td>0.03082</td>
</tr>
<tr>
<td>9</td>
<td>27</td>
<td>0.02833(10)</td>
<td>0.90</td>
<td>61%</td>
<td>0.02723</td>
</tr>
<tr>
<td>9</td>
<td>30</td>
<td>0.02355(11)</td>
<td>1.16</td>
<td>27%</td>
<td>0.02427</td>
</tr>
<tr>
<td>9</td>
<td>36</td>
<td>0.01888(13)</td>
<td>0.98</td>
<td>48%</td>
<td>0.01959</td>
</tr>
<tr>
<td>10</td>
<td>18</td>
<td>0.03127(47)</td>
<td>0.44</td>
<td>99%</td>
<td>0.03119</td>
</tr>
<tr>
<td>10</td>
<td>20</td>
<td>0.02670(61)</td>
<td>1.01</td>
<td>45%</td>
<td>0.02710</td>
</tr>
<tr>
<td>10</td>
<td>22</td>
<td>0.02339(34)</td>
<td>0.88</td>
<td>64%</td>
<td>0.02374</td>
</tr>
<tr>
<td>10</td>
<td>24</td>
<td>0.02049(46)</td>
<td>0.79</td>
<td>75%</td>
<td>0.02092</td>
</tr>
<tr>
<td>10</td>
<td>26</td>
<td>0.01960(47)</td>
<td>1.02</td>
<td>44%</td>
<td>0.01854</td>
</tr>
<tr>
<td>10</td>
<td>28</td>
<td>0.01644(70)</td>
<td>0.83</td>
<td>69%</td>
<td>0.01650</td>
</tr>
<tr>
<td>10</td>
<td>30</td>
<td>0.01473(88)</td>
<td>0.84</td>
<td>80%</td>
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</tr>
<tr>
<td>11</td>
<td>20</td>
<td>0.02024(75)</td>
<td>1.17</td>
<td>25%</td>
<td>0.02049</td>
</tr>
<tr>
<td>11</td>
<td>22</td>
<td>0.01766(78)</td>
<td>1.05</td>
<td>39%</td>
<td>0.01735</td>
</tr>
<tr>
<td>11</td>
<td>24</td>
<td>0.01495(61)</td>
<td>0.77</td>
<td>77%</td>
<td>0.01479</td>
</tr>
<tr>
<td>11</td>
<td>26</td>
<td>0.01292(69)</td>
<td>0.67</td>
<td>84%</td>
<td>0.01267</td>
</tr>
<tr>
<td>11</td>
<td>28</td>
<td>0.01024(91)</td>
<td>0.66</td>
<td>87%</td>
<td>0.01090</td>
</tr>
<tr>
<td>11</td>
<td>32</td>
<td>0.00782(12)</td>
<td>0.85</td>
<td>73%</td>
<td>0.00815</td>
</tr>
</tbody>
</table>

**Tab. 1.** The values of $E$ are reported with the $\chi^2$ per degree of freedom and the confidence levels, as obtained from the fit of $G(k)$ with formula (14). The values in the last column are obtained from the best fit of all data to formula (9). The same data are plotted in Fig. 4.
Fitting our results for the energy gaps $E$ with the CWM formula (9) we obtain the following values of the interface tension and of the constant:

$$\sigma = 0.009912(75)$$
$$\delta = 0.1377(19)$$

with a $\chi^2$ per degree of freedom and a confidence level

$$\chi^2 = 0.73 \quad \text{C.L.} = 82\% \quad (17)$$

thus confirming the accuracy of the CWM. In Tab. 1 the MC results for $E$ are compared with the predictions of formula (9) in which the best-fit values of $\delta$ and $\sigma$ have been substituted. This comparison is represented graphically in Fig. 4.

The importance of the inclusion of the two-loop contributions can be seen by fitting the MC data with the classical formula

$$E(R, T) = \delta \: e^{-\sigma RT} \quad (18)$$

and with the one-loop approximation ($R \geq T$)

$$E(R, T) = \delta \: e^{-\sigma RT} \: \frac{Z_q^{(1\:\text{loop})}(R)}{Z_q^{(1\:\text{loop})}(1)}. \quad (19)$$

In the former case we obtain $\chi^2$/d.o.f. = 36.3, in the latter $\chi^2$/d.o.f = 3.60: the two-loop correction must be included to obtain a good agreement with numerical data.

We have already noted that the two-loop corrections affect the value of $E$ also for symmetric ($T = R$) lattices (cfr. (10)), in contrast to what happens for the scale-invariant one-loop contribution (5) [4]. Indeed, the importance of including two-loop corrections can be seen by fitting only the energy gaps $E$ obtained on symmetric lattices ($T = R$): using the two-loop expression (10) we obtain $\chi^2 = 0.79$, while the classical formula (11) gives $\chi^2 = 1.48$. The results of all these fits are summarized in Tab. 2.

We would like to stress the remarkable stability of the results obtained with the two-loop approximation fitting all the data or only the symmetric ones. This can be seen comparing the values of $\sigma$ and $\delta$ given in the first and fourth line of Tab. 2.
<table>
<thead>
<tr>
<th>Data</th>
<th>Approx.</th>
<th>$\sigma$</th>
<th>$\delta$</th>
<th>$\chi^2$</th>
<th>C.L.</th>
</tr>
</thead>
<tbody>
<tr>
<td>all</td>
<td>2–loop</td>
<td>0.009912(75)</td>
<td>0.1377(19)</td>
<td>0.73</td>
<td>0.82</td>
</tr>
<tr>
<td>all</td>
<td>1–loop</td>
<td>0.010053(75)</td>
<td>0.1724(23)</td>
<td>3.60</td>
<td>0.00</td>
</tr>
<tr>
<td>all</td>
<td>class.</td>
<td>0.008092(75)</td>
<td>0.1395(19)</td>
<td>36.3</td>
<td>0.00</td>
</tr>
<tr>
<td>$T = R$</td>
<td>2–loop</td>
<td>0.00981(14)</td>
<td>0.1361(26)</td>
<td>0.79</td>
<td>0.53</td>
</tr>
<tr>
<td>$T = R$</td>
<td>class.</td>
<td>0.01075(14)</td>
<td>0.1866(36)</td>
<td>1.48</td>
<td>0.20</td>
</tr>
<tr>
<td>$T = 11$</td>
<td>2–loop</td>
<td>0.00997(69)</td>
<td>0.140(24)</td>
<td>0.26</td>
<td>0.90</td>
</tr>
<tr>
<td>$T = 11$</td>
<td>1–loop</td>
<td>0.00965(69)</td>
<td>0.151(26)</td>
<td>0.22</td>
<td>0.92</td>
</tr>
</tbody>
</table>

**Tab. 2.** Results of the fit of $E$ with two–loop, one–loop and classical approximations of the CWM, considering all values of $(R,T)$, symmetric $(R,R)$ lattices or $(R,T=11)$ lattices.

On the other hand, the result obtained using the classical formula (18) is not compatible with the previous ones even using only the symmetric data, as it is shown in the fifth line of the same table. The best fit curve obtained from (18) in the latter case is plotted in Fig. 5 were also the "asymmetric" MC data are reported for comparison.

We would also like to observe that a good agreement with the one–loop approximation of the CWM can be obtained [4] if one considers low values of ratios $z = R/T$ and high values of the minimal area $A_m = RT$, i.e. where the two–loop contribution (6) are maximally suppressed. This is show in the last two lines of Tab. 2 and in Fig.6.

### 4 Conclusions

In this paper we have shown that the CWM in the two–loop approximation provides an excellent description of order–order interfaces in the 3D three–state Potts model. This result, together with the corresponding one for the 3D Ising model [4], strongly supports the hypothesis of the universality of the CWM description of interface physics in 3D statistical models.

It is worth stressing again that the CWM corrections (9) to the finite–size behavior of the interface free energy do not introduce any new free parameters with respect to the "classical" picture (18).

Besides the intrinsic physical interest of this picture, it should be noted that the CWM provides an accurate description of finite–size corrections to the free energy of rough interfaces, thus enabling one to extract correct
informations about physical observables from finite lattices of different geometries, as it has been recently shown [21].

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References


Figure Captions

Fig. 1. Histogram of the real part of the magnetization for a typical MC ensemble (in this case $T = 20, R = 20$). The absence of a peak in $\text{Re } M = 0$ indicates that the disordered phase does not coexist with the ordered ones at our $\beta = 0.3680$.

Fig. 2. Distribution of a sample of 5,000 configurations generated by the MC simulation in the complex plane of the magnetization for a lattice $T = R = 18$. The three clusters of points represent the one–phase configurations; the straight lines joining the clusters are the two–interface configurations.

Fig. 3. The same of Fig. 2 for a lattice $T = 10, R = 20$. The three-interface configurations are uniformly distributed in the interior of the triangle.

Fig. 4. Comparison of the predictions of the CWM with the MC data: the energy gap $E$ is plotted as a function of $z = R/T$. The lines represent the best fit of all data to formula (9): from up to down they correspond respectively to $T = 9, 10, 11$ fixed (cfr. Tab. 1).

Fig. 5. Comparison of the predictions of the classical formula with the MC data: $E$ is plotted as a function of $A_m = RT$. The line represent the best fit of the symmetric $T = R$ data, reported with error bars, to formula (18); the asymmetric MC data are also reported: squares correspond to $T = 9$ data, circles to $T = 10$ and diamonds to $T = 11$.

Fig. 6. Comparison of the predictions of the two–loop (9) and one–loop (19) approximations for the $T = 11$ data, with $z = R/T$. The dashed line represent the one–loop best fit while the two–loop is the dotted line.