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LETTER TO THE EDITOR

A novel method of calculating amplitude ratios by series expansions

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Abstract. We introduce a new method of calculating critical amplitude ratios using series, which is both simple and powerful. This method, which gives estimates for the amplitude ratios that are neither biased by the values of the critical points nor by the critical exponents, is applied to several models. We show that this method produces results where no reliable estimates from series expansion exist. In particular we find 0.025 ± 0.001 for $A\Gamma'/B^2$ for the 3D Ising model and 220 ± 10 for C^+/C^- for the two-dimensional percolation model in agreement with, and with more accuracy than, values obtained by other methods.

The concept of universality plays a crucial role in the study of critical phenomena (for a review see Aharony 1976). It means that apparently different physical systems, which belong to the same universality class, share the same physical characteristics near the phase transition. Most of the extensive work in the field of critical phenomena was applied to calculate the universal critical exponents using renormalisation group calculations, series expansions, Monte Carlo simulations and experiments (for a review see Domb and Green 1972–6). Though it was well known (see, e.g., Aharony and Hohenberg 1976 and references therein) that amplitude ratios also exhibit universal behaviour, far fewer estimates of the amplitude ratios exist in the literature, mainly due to the fact that the only available method of estimating the amplitude ratios involved estimating the individual amplitudes. Thus one had to estimate first the critical points in order to have an estimate for the amplitude.

Amplitude ratios should be studied especially when the critical exponents do not suffice to clear the question of different universality classes. For example, in the case of Anderson localisation (for a review see, e.g., Lee and Ramakrishnan 1985), the question of different universality classes is not yet clear and studying amplitude ratios (like $\sigma/(\omega\varepsilon)_0$, where σ is the conductivity and $(\omega\varepsilon)_0$ is the limit of $\omega\varepsilon(\omega)$ as ω approaches zero) might shed some light upon this question. Amplitude ratios could also be used in other problems such as liquid crystals (see, e.g., Martinez-Miranda *et al* 1986), superconductivity in disordered systems (see, e.g., Goldman and Wolf 1985), random field Ising models (Aharony *et al* 1985), etc, where the question of universality is not yet resolved.

The method of series expansions has been used extensively and successfully in the study of critical phenomena (for a review see Domb and Green 1974). However, most of the studies obtained estimates for the critical points and the critical exponents. Only when these were known with high accuracy (often from other sources), could one estimate the amplitudes. Recently, Adler *et al* (1986, hereafter referred to as AAMH)

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used series to directly calculate several amplitude ratios for the percolation problem. However, their method still depends on the value of the critical point, though one does not have to calculate the critical exponents. In this letter we propose a new method of calculating amplitude ratios, where one uses the given series to create a new series. This method has the following advantages.

(i) One does not have to know the critical point nor the critical exponents.

(ii) The new series to be analysed has the asymptotic behaviour $S/(1-x)$, where x is the expansion parameter and S is related to the amplitude ratio, no matter what the values of the critical point or the critical exponents for the original problem were. Therefore one has a good way of estimating how good the approximation is: the closer the pole to $x=1$, the closer the residue to the wanted ratio S.

(iii) The resulting series do not have, to a leading order, any corrections to scaling (at least to first order in ε), which means that the estimates are more reliable.

Using this new method we obtained estimates for amplitude ratios, where no results or very poor results have been obtained previously, using series expansions. In particular we find that for the 3D Ising model the ratio $A'\Gamma'/B^2$ (where A', B and Γ' are the low-temperature amplitudes of the specific heat, spontaneous magnetisation and magnetic susceptibility, respectively) is 0.025 ± 0.001 in agreement with the ε expansion method and with the values of the individual amplitudes obtained by different methods. We also find $C^+/C^-=220\pm10$ (where C^+/C^- is the low(high) concentration amplitude of the mean size of the clusters) for the two-dimensional percolation problem, in agreement with and more accurate than the results of the Monte Carlo calculations and contrary to previous series calculations.

Let us assume that one constructed series for some physical quantities χ_k as a function of some physical parameter x:

$$\chi_k(x)=\sum_{n=0}^{N} a_{kn}x^n. \tag{1}$$

All the χ_k are expected to diverge at the same x_c with the asymptotic forms

$$\chi_k(x)\simeq A_k(x_c-x)^{-\gamma_k}. \tag{2}$$

The universality of the amplitude ratios means that, if the relation $\Sigma_i\,\gamma_{k_i}=\Sigma_j\,\gamma_{l_j}$ holds, then the ratio

$$R(k_i,l_j)=\prod_i A_{k_i}\left(\prod_j A_{l_j}\right)^{-1} \tag{3}$$

may be universal if the χ_k are normalised properly. We would like to evaluate this ratio from the series coefficients (1).

For example, if the exponents $2-\alpha$, β and γ correspond to the free energy, magnetisation and magnetic susceptibility, respectively, the relation $2-\alpha=\gamma+2\beta$ holds. This corresponds to $\gamma_1=2-\alpha$, $\gamma_2=\beta$ and $\gamma_3=-\gamma$ above, such that $k_1=1$, $k_2=3$, $l_1=2$ and $l_2=2$. Therefore, the ratio A_1A_2/A_3^2 is universal and relates to $A'\Gamma'/B^2$ in the usual notation.

The AAMH method was to study the series $\Pi_i\,\chi_{k_i}(x)/\Pi_j\,\chi_{l_j}(x)$. This series should be regular at x_c, so one can approximate the new series by a rational function and obtain approximants for the amplitude ratio by evaluating the rational approximants at x_c. The problems of this method are as follows.

(i) The value of the approximant depends on x_c.

(ii) Since the series do not show any critical behaviour, there is no way of finding out how good the approximants are.

(iii) It is very hard to estimate the error of this procedure.

(iv) It is known from the study of series expansions that multiplying and dividing series give rise to less well behaved series.

The new method we propose is very simple. We construct a new series:

$$\Phi_{(k_i,l_j)}(x)=\sum_{n=0}^{N}\frac{\Pi_i\, a_{k_in}}{\Pi_j\, a_{l_jn}}x^n\equiv\sum_{n=0}^{N}B_n x^n. \tag{4}$$

Expanding (2) in powers of x one finds

$$a_{kn}\simeq A_i x_c^{-\gamma_k}\frac{\Gamma(\gamma_k+n)}{\Gamma(\gamma_k)\Gamma(n+1)}\frac{(-1)^n}{x_c^n} \tag{5}$$

where Γ is the gamma function. Using Stirling's formula one has

$$B_n\simeq\frac{\Pi_i A_{k_i}}{\Pi_j A_{l_j}}\frac{\Pi_j\,\Gamma(\gamma_{l_j})}{\Pi_i\,\Gamma(\gamma_{k_i})} \tag{6}$$

to first order in $1/n$, which leads to the asymptotic behaviour

$$\Phi_{(k_i,l_j)}(x)\simeq\frac{R(k_i,l_j)\Pi_j\,\Gamma(\gamma_{l_j})/\Pi_i\,\Gamma(\gamma_{k_i})}{1-x}\equiv\frac{S(k_i,l_j)}{1-x}. \tag{7}$$

Thus we obtained a very simple series which diverges at $x=1$ with an exponent equal to unity, no matter what the values of the original critical point or critical exponents were. Furthermore, one can also calculate the first correction term to the series (5) due to the correction to scaling terms for the original series (1). Since, at least to first order in ε, all the corrections to scaling exponents are the same and their respective amplitudes are linear functions of γ_k (see, e.g., Aharony and Ahlers 1980), then one can show that the first correction to scaling terms cancel and the series (5) will have less important correction to scaling terms than the original series.

Now in order to calculate S one can use any of the many methods devised to analyse series (see, e.g., Domb and Green 1974). For example, one can approximate the new series by rational functions, choose those approximants that give a pole near $x=1$ and evaluate the residue as an approximant for S. An even simpler method is to estimate S by extrapolating B_n to infinite n or by extrapolating $(nB_n-(n-k)B_{n-k})/k$ for various values of k, etc.

Though we have constructed an approximant for $S(k_i, l_j)$, there is no *a priori* justification for preferring $R(k_i, l_j)$ as the wanted ratio. Both these ratios are universal, but there is no known way of calculating R from series without calculating first the critical exponents, while we have demonstrated above how to calculate S directly, so S may serve as an independent universal quantity. In the rest of this letter, we apply our method to several problems and calculate S. Our values are compared with other results.

First, as a check, we apply the method to the two-dimensional Ising model and calculate the amplitude ratio S that relates to the ratio $A'\Gamma'/B^2$, where A, B and Γ are defined above, where we have used the series published by Sykes *et al* (1973b) for various lattices. Our method gives rise to the estimate $S=0.700\pm0.005$, while the exact result (see McCoy and Wu 1973, Barouch *et al* 1973) is 0.699.

The first application served merely as a check since other methods were used to estimate this ratio with very good accuracy, especially since the critical temperature and the critical exponents are known analytically. The situation for the 3D Ising model is, on the other hand, completely different. No exact results are known and the low-temperature series are very hard to analyse. Analysis of these series, especially the specific heat series, could only lead to the conclusion that the results for the exponents do not contradict universality but no reliable estimates for the exponents from low temperature series exist (see, e.g., Domb and Green 1974). Moreover, since all the earlier known methods for estimating the amplitudes from series depended on the values of the exponents then the estimates, for example, for the amplitude of the low temperature specific heat A' differ by a factor of three, depending on the exact value of the exponent used (Gaunt and Domb 1968). We applied the AAMH method to the series derived by Sykes *et al* (1973a) for four lattices; diamond, simple cubic, BCC and FCC in order to calculate $A'\Gamma'/B^2$. This method did not give any consistent results and different Padé estimates gave different results.

Next, we used our method to analyse the series. While the coefficients for the diamond lattice were very regular, the other series had other singular points besides the physical one. In order to decrease the singularity of the unphysical point we multiplied all the series by $1-p/p^*$, where p^* is the approximate location of the unphysical singular point. This procedure is not sensitive to the value of p^* employed and changes of 10% in the values of p^* result in less than a 1% change in the value of the amplitude ratio. In table 1 we show the last six terms B_n of the resulting series (4) and also the series $(nB_n-(n-2)B_{n-2})/2$ which serves as another approximant for S. One can see that the B_n are decreasing monotonically, while the $(nB_n-(n-2)B_{n-2})/2$ are practically constant for the diamond and simple cubic lattices and erratic for the other two lattices. One can also see that the odd and even terms form a smooth function and extrapolating this function to infinite n gives rise to the estimate $S=0.45\pm0.02$, which is consistent with the constant values of $(nB_n(n-2)B_{n-2})/2$. One can combine the ε expansion for various amplitude ratios (Aharony and Hohenberg 1976) with the ε expansion for the exponents (see, e.g., Domb and Green 1976, p 319) to get an ε expansion for S, which to first order in ε gives the estimate $S=0.5\pm0.3$ (the error bar for the ε expansion was obtained using different Padé estimates). Combining the most reliable estimates for the individual amplitudes from the equation of state method (Barmatz *et al* 1975) and series (Guttmann 1975, Essam and Hunter 1968) gives the estimate $S=0.45$. One should note, however, that the literature values for the amplitudes obtained by series should be taken with caution, since they were obtained by methods which are biased by the values of the critical exponents and the values of the exponents used in the above references are different from recent estimates of these exponents (see, e.g., Adler *et al* 1982, Adler 1983) by 5%. One can translate

Table 1. Last six B_n and $(nB_n-(n-2)B_{n-2})/2$ for 3D Ising model.

Lattice	N	B_n	$(nB_n-(n-2)B_{n-2})/2$
DM	14	0.5768, 0.5590, 0.5444, 0.5329, 0.5237, 0.5175	0.4552, 0.4448, 0.4150, 0.4156, 0.4202, 0.4328
SC	17	0.5723, 0.5649, 0.5478, 0.5446, 0.5310, 0.5304	0.4266, 0.4428, 0.4376, 0.4428, 0.4383, 0.4452
BCC	14	0.8136, 0.7028, 0.6274, 0.7329, 0.5432, 0.5619	0.5885, 0.4197, −0.2102, 0.8830, 0.0803, −0.4634
FCC	22	0.7694, 0.7660, 0.6178, 0.6625, 0.6511, 0.6196	1.386, 1.176, −0.6703, −0.2685, 0.9677, 0.1907

all these results, using the recent estimates of the exponents, to get an approximant for $A'\Gamma'/B^2$. The ε expansion gives $R=0.025$, the combined literature amplitude estimates give $R=0.024$, while our method gives the value $R=0.023\pm0.001$.

So far we have dealt with amplitude ratios of quantities on the same side of the transition. One can also discuss amplitude ratios from the two sides of the transition. However, in this case the method loses some of its main advantages. In order to use this method the series have to diverge at the same point, so one has to multiply each term in one of the series by the ratio x_{c1}/x_{c2} to the appropriate power, where x_{c1} and x_{c2} are the two critical points (e.g. $\exp(-2J/KT_c)$ and $\tanh(J/KT_c)$ for the Ising model). Thus one has to know the critical threshold to very good accuracy. It seems from analysis of some models that the results are rather sensitive to the value of the critical point and a change of 1% in this value may lead to a change of 10% in the estimate of the amplitude ratio. Also, the first correction to scaling term will not drop out. In spite of all this the method still has some advantages over that used previously, namely calculating explicitly the individual amplitudes after calculating the critical points and critical exponents, since the analysis does not depend on the value of the critical exponents.

Having checked that the method gave the known results from the 2D Ising model, we applied it to the 2D percolation model in order to calculate the ratio C^+/C^-, where $C^+(C^-)$ is the low(high) concentration amplitude of the mean size of the clusters. There were various estimates for this ratio which varied from the order of 200 (Hoshen *et al* 1979, Nakanishi and Stanley 1980, Monte Carlo simulation), of the order of 10 (Aharony 1980, ε expansion) and of the order of unity (Sykes *et al* (1976), series expansion by calculating the individual amplitudes). We applied our method to the series published by Sykes *et al* (1976) for the square, triangular and honeycomb lattices (bond percolation) and the triangular lattice (site percolation). As mentioned above, one first has to factorise one of the series, so that both of them would diverge in the same point. Since the critical concentrations for those problems are known exactly this procedure does not produce any problems. Carrying on our procedure we find

228 ± 12 (triangular, site percolation) 175 ± 50 (triangular, bond percolation)

215 ± 30 (square, bond percolation) 219 ± 4 (honeycomb, bond percolation)

in agreement with the Monte Carlo results, 196 ± 40 (Hoshen *et al* 1979) and 219 (Nakanishi and Stanley 1980) and with the extrapolation of the scaling function for the cluster size distribution from the series data, $180\pm20\%$ (Wolff and Stauffer 1978).

To conclude, we have introduced a new method of calculating amplitude ratios and shown how it can be applied to problems where no reliable series estimates exist. Apart from the application of this new method to the problem mentioned above, this method was applied in order to estimate amplitude ratios as part of intense investigations of other problems such as the diluted resistor network (Meir *et al* 1987a), diffusion on percolation clusters (Meir *et al* 1987b), etc.

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