J. Phys. A: Math. Gen. **15** (1982) L405–L412. Printed in Great Britain

LETTER TO THE EDITOR

Site percolation threshold for honeycomb and square lattices

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Received 18 May 1982

Abstract. A new method of estimating the critical percolation threshold is proposed, based on Stauffer's cluster number scaling hypothesis and the universality with respect to lattice structure of the corresponding Stauffer scaling function. This method is illustrated by obtaining estimates of the site percolation threshold for the honeycomb lattice, $p_c = 0.6962 \pm 0.0006$, and for the square lattice, $p_c = 0.5923 \pm 0.0007$. The error bars or 'confidence limits' of our estimates are substantially smaller than previous series estimates, and—for the honeycomb lattice—would have to be multiplied by the factor 18 to include the value, $p_c = 2^{-1/2}$, recently proposed by Kondor to be exact. An additional result is $R = 4.95 \pm 0.15$, where $R = \lim_{s\to\infty} R_s$, and R_s is the ratio of the cluster number scaling function at its maximum to its value at p_c for clusters of size s.

Studies of percolation phenomena are of interest not only for their potential utility in understanding a range of physical phenomena where connectivity is a dominant feature, but also because the geometric critical phenomena exemplified by percolation possess many striking parallels with the thermal phenomena exemplified by the Ising model. Despite the apparent simplicity of percolation, comparatively few exact results are known, even for a two-dimensional system; e.g. there is no analogue in percolation of the Onsager solution of the zero-field Ising model. In fact, the percolation threshold p_c is known exactly for only four cases: triangular lattice site percolation (TS), triangular lattice bond percolation (TB), honeycomb lattice bond percolation (HB), and square lattice bond percolation (SB). Therefore, considerable interest has arisen as a result of a recent letter by Kondor (1980), which produces an argument supporting the possibility that the site percolation threshold for the honeycomb lattice is given by the simple relation

$$p_c = 2^{-1/2} = 0.707107\ldots. \tag{1}$$

Kondor's exact value lies slightly outside the most reliable current series estimates (Sykes *et al* 1976), $p_c = 0.698 \pm 0.003$, obtained from extrapolations to $s = \infty$ (e.g. by Padé approximants) of low-density series expansions, which are calculated to a finite order by exact enumeration of finite clusters up to site size $s = 20$. However since the 'error bars' are, in reality, somewhat subjective 'confidence limits,' it seemed quite possible that Kondor *could* be right if the confidence limits were made larger by a factor of three. Higher-precision numerical work is called for to test the possible

† Supported in part by grants from ARO, ONR, and NSF.

validity of his exact result more reliably, and the present letter is a response to this need. Specifically, we propose a new method of estimating the site percolation threshold. We first present the method and then use it to calculate p_c for the honeycomb lattice. We shall see that the necessary increase in precision is indeed obtained, the new estimates we present being about five times more precise than previous estimates. This increased precision strongly suggests that Kondor's 'exact value' is not correct (see also Enting and Wu 1982). We also show that the method works for the square lattice, and obtain an estimate whose confidence limits are also about five times smaller than those of previous estimates based on low-density expansions (Sykes *et al* 1976).

Our method has as its starting point the assumed validity of the cluster number scaling hypothesis (Stauffer 1975, 1979): for sufficiently small values of $\varepsilon \equiv (p_c - p)/p_c$ and $1/s$, the mean number of s-site (or s-bond) clusters per lattice site, $n(s, p)$, obeys the asymptotic relation

$$n(s, p) \sim s^{-\tau} f_0(\varepsilon s^{\sigma}). \tag{2}$$

Here σ and τ are critical exponents related to the usual percolation exponents through $\sigma = 1/\beta\delta$ and $\tau = 2 + 1/\delta$. The validity of (2) has been tested for small s by exact enumeration methods (Stauffer 1975), and for large s by Monte Carlo simulations (Hoshen *et al* 1979, Nakanishi and Stanley 1980, 1981). Moreover, the scaling function $f_0(x)$ defined in (2) has been found to be 'universal' in that it depends only on system dimensionality ($d = 1, 2, \ldots$) and not on the individual lattice type.

Stauffer (1979) has focused attention on the ratio

$$R_s \equiv n(s, p_{\max})/n(s, p_c) \tag{3a}$$

where $p_{\max}(s)$ is the value of p for which $n(s, p)$ achieves its maximum value for fixed s (figure 1(a)), and on the limiting value

$$R = \lim_{s \to \infty} R_s. \tag{3b}$$

As $s \to \infty$, $p_{\max}(s) \to p_c$, and we expect from (2) and (3) that

$$R = f_0(x_{\max})/f_0(0) \tag{4}$$

where $x_{\max}$ is the value of x for which the scaling function $f_0(x)$ achieves its maximum. If the scaling function $f_0(x)$ is universal, then the Stauffer ratio R is *also* universal.

For $1 < d < \infty$, R_s can be calculated exactly *only* for small s and *only* for those four two-dimensional systems for which p_c is known exactly: TS, TB, HB, and SB. The requisite functions $n(s, p)$ are calculated in Sykes and Glen (1976) and in Sykes *et al* (1981). By extrapolating the small-s values of R_s to infinite s, Wolff and Stauffer (1978) estimate $R = 4.8$. Stoll and Domb (1979) estimated $R = 5.4$ while Hoshen *et al* (1979) estimated $R = 4.8$ by using Monte Carlo methods to estimate R_s for larger s—thereby facilitating the $s = \infty$ extrapolation of (3b) at the price of non-exact, and hence much less reliable, values of R_s. Our own estimates of R, presented below, are consistent with these previous estimates: if the correction-to-scaling exponent is in the range 0.5–0.7, then R is in the range 4.95 ± 0.15 (3% accuracy).

If p_c is *not* known exactly, the functions R_s are difficult to estimate since $n(s, p)$ varies rapidly in the vicinity of p_c. Thus R_s, and hence also R, are sensitive functions of the assumed threshold p_c^{trial}. What at first sight might seem to be a disadvantage is actually quite fortunate: if we can estimate R with an accuracy of 3%, we can

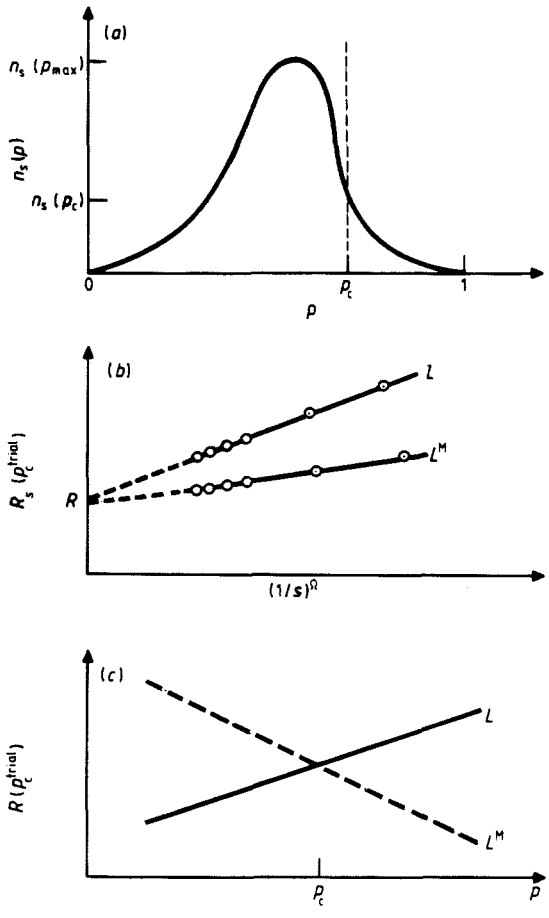

Figure 1. (*a*) Schematic behaviour of the $n(s, p)$, the number of s-site clusters per lattice site, indicating the crucial quantities entering into the calculation of the Stauffer ratios $R_s = n(s, p_{max})/n(s, p_c^{trial})$. (*b*) Schematic plot of the Stauffer ratio R_s against $(1/s)^{\Omega}$ for an arbitrary lattice L and its match L^M. (*c*) Behaviour of the limiting Stauffer ratio R defined in (4) plotted against p_c^{trial} for lattices L and L^M.

determine p_c to an accuracy of much better than 0.1% by varying p_c^{trial} until $R(p_c^{trial}) \cong R$ (figure 1(*b*)). Moreover, we have noted that the dependence of R on p_c^{trial} for certain pairs of lattices has opposite sign (figure 1(*c*)). These are matching lattices, for which we know (Sykes and Essam 1974)

$$p_c + p_c^M = 1. \tag{5}$$

Hence the point of intersection of the two curves represents the true p_c, which can thereby be determined quite accurately.

We now turn to the actual method of extrapolating the calculated values of R_s to $s = \infty$. We may be guided by the expected† form of the leading finite-s correction

† See Margolina *et al* (1982) for more discussion of the form of equation (6).

(Nakanishi and Stanley 1980) to the asymptotic scaling relation (2)

$$n(s,p) \sim s^{-\tau}[f_0(x)+s^{-\Omega}f_1(x)+\ldots] \sim s^{-\tau}f_0(x)[1+s^{-\Omega}c(x)+\ldots] \tag{6}$$

where $x \sim \varepsilon s^{\sigma}$, $c(x) \equiv f_1(x)/f_0(x)$ and Ω is termed the 'correction-to-scaling' exponent. Substituting (6) into (3*a*), we find

$$R_s = R[1+c(x_m)s^{-\Omega}+\ldots]/[1+c(0)s^{-\Omega}+\ldots] = R\{1+[c(x_m)-c(0)]s^{-\Omega}+O(s^{-2\Omega})\}. \tag{7}$$

The form of (7) suggests plotting R_s against $s^{-\Omega}$. If the coefficient of the $s^{-\Omega}$ term is significantly larger than the coefficient of the $s^{-2\Omega}$ term, then the points R_s should fall roughly on a straight line which may then be extrapolated to $s=\infty$ to obtain a reliable estimate for R.

It should be emphasised that the value of R depends on the value we assumed for Ω (figure 2). Uncertainty in Ω is the major cause for relatively broad range of R (4.8–5.1). Unfortunately it was hard to reduce the uncertainty in (0.5–0.7) since we work with small values of s where higher-order terms in $s^{-\Omega}$ play an important role. Note also that $A=c(x_m)-c(0)$ is not a universal quantity and can even be very close to zero. That would make the $s^{-2\Omega}$ term dominant; i.e. the apparent Ω could be equal to 2Ω. Also, other irrelevant fields with different Ω can be important for our range of s.

Figure 3 shows such plots for the honeycomb site (HS) and honeycomb matching site (HMS) problems. In 3(*a*), $p_c^{\text{trial}}=0.6962$, which is the value of p_c^{trial} for which the extrapolated value of R for HS is closest to R for HMS. In 3(*b*), $p_c^{\text{trial}}=0.701$, the largest value allowed by the confidence limits set by the most reliable previous estimates, $p_c=0.698\pm0.003$, obtained by Sykes *et al* (1976) using Padé approximants to low-density expansions. In 3(*c*), $p_c^{\text{trial}}=0.707$, the Kondor conjecture. It is clear that the present method is very sensitive indeed to p_c^{trial}.

In figure 3, the correction-to-scaling exponent Ω is taken to be 0.6, which is roughly an average of previous literature estimates (the exponent Ω is notoriously difficult to evaluate—see e.g. the discussion in Stauffer (1979) and references therein, especially Gaunt and Sykes (1976), Houghton *et al* (1978), Hoshen *et al* (1979), Nakanishi and Stanley (1980), Margolina *et al* (1982) and Adler *et al* (1982).

To determine how sensitively our estimate of p_c depends on the choice of Ω, we have calculated $R(p_c^{\text{trial}})$ for several values of Ω, and the results for $\Omega=0.5$, 0.6, and 0.7 are shown in figure 4. We see that the conclusion that the best choice of p_c^{trial} is 0.69615 is remarkably independent of the choice of Ω.

To give confidence limits on our estimate $p_c=0.6962$, we must ascertain the accuracy with which the sequences $R_s(p_c^{\text{trial}})$ can be extrapolated to $s=\infty$. Therefore we plotted the corresponding values of $R_s(p_c)$ for the four two-dimensional percolation problems for which p_c is known exactly (TS, TB, HB and SB) for a range of Ω_{trial}.

The limiting values of R vary slightly from lattice to lattice, giving us a measure of the 'confidence limits' that one can place on estimates of R. More important is the fact that the estimate R depends on the assumed value of the correction-to-scaling exponent Ω, which is also apparent from figure 4. However for each possible value of Ω, analysis of the four lattices for which p_c is known exactly gives rise to a fairly narrow range of permissible values of R—roughly $\pm3\%$. Accordingly, we can interpret

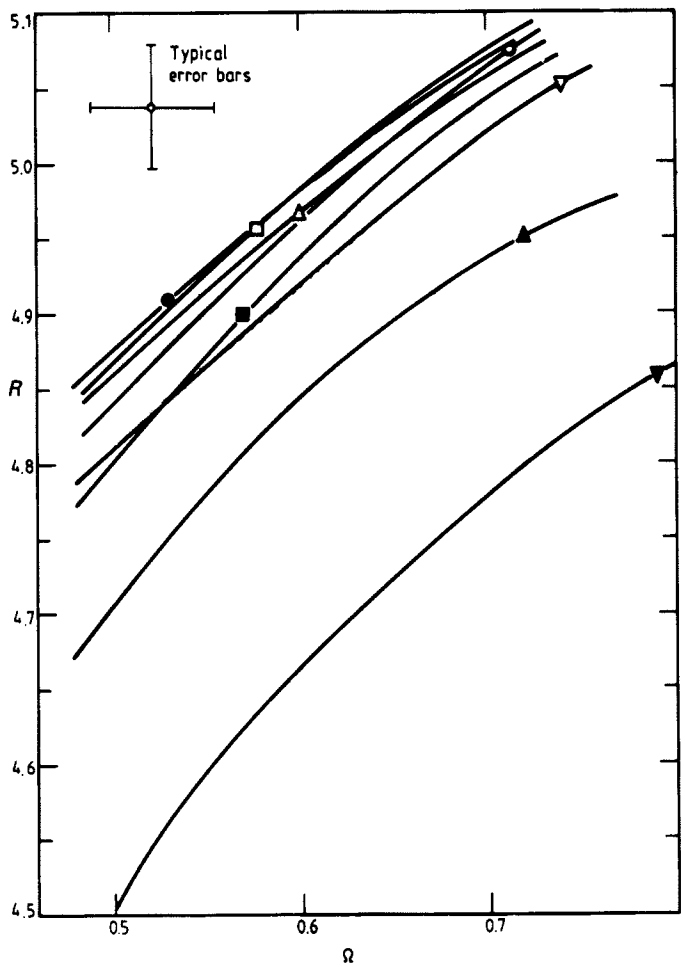

Figure 2. We have calculated R_s as a function of $s^{-\Omega}$ for the eight $d=2$ cases studied: ▽, honeycomb bond; △, honeycomb site; ○, honeycomb match, ▲, square bond; ●, square site; □, square match; ▼, triangular bond; ■, triangular site. The extrapolated values R for these lattices as functions of trial value Ω are given in this figure, indicating our most effective values Ω_{eff} for each lattice: values of Ω far from Ω_{eff} (for every lattice) produce curved plots with less accurate extrapolation for R. The range of acceptable values of Ω, around Ω_{eff} for a certain lattice is set by eliminating values of Ω which produce appreciably curved plots. For such a range of uncertainty in Ω, depicted by horizontal error bars, there corresponds an uncertainty in the respective value of R. This latter uncertainty is typically 1% for each lattice and weakly depends on Ω. We further assumed that the true, universal value R lies in the range determined by the union of the individual uncertainties for all analysed lattices, giving $R=4.95\pm0.15$, so that the confidence limits on R are ±3%.

the straight lines in figure 4 as having an accuracy of 3%. This determines the confidence limits on p_c to be

$$p_c = 0.6962 \pm 0.0006 \qquad \text{(honeycomb)}. \tag{8a}$$

Note that in order to include the Kondor conjecture, the confidence limits of our

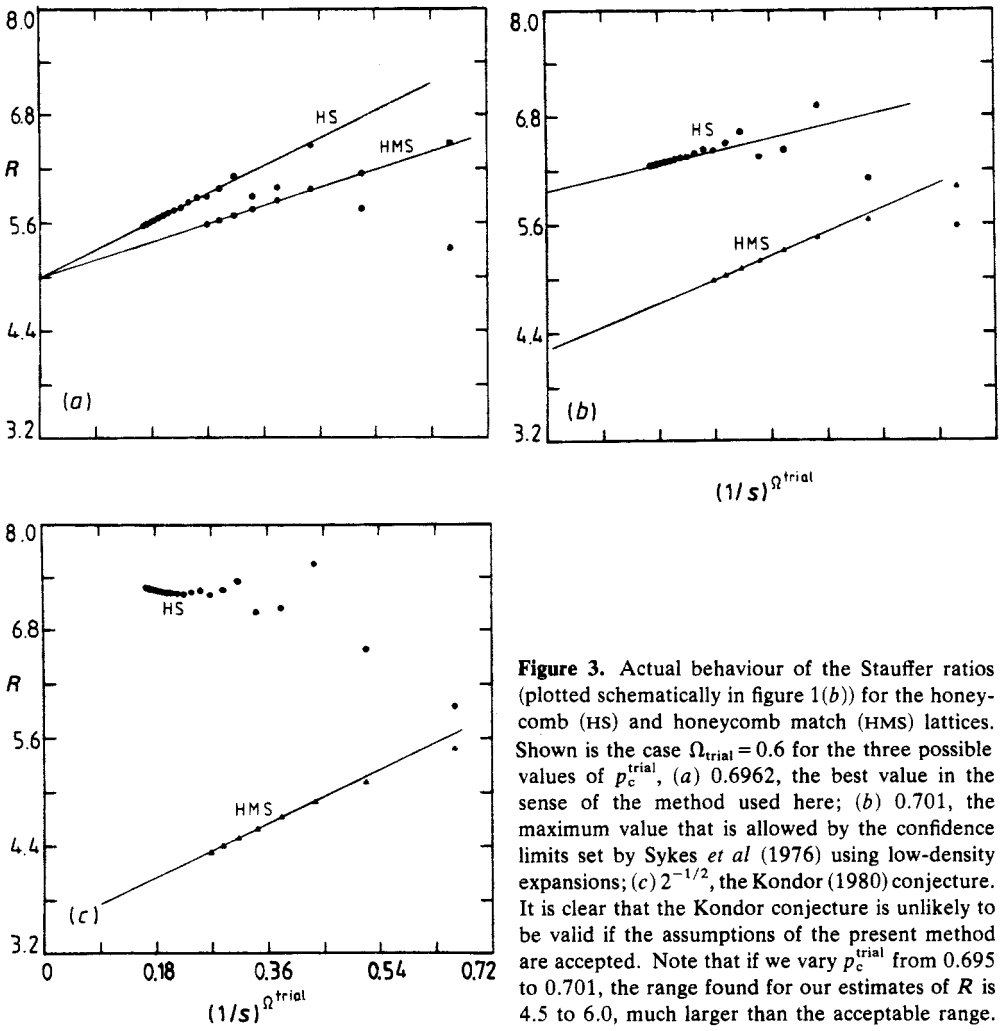

Figure 3. Actual behaviour of the Stauffer ratios (plotted schematically in figure 1(*b*)) for the honeycomb (HS) and honeycomb match (HMS) lattices. Shown is the case $\Omega_{trial} = 0.6$ for the three possible values of p_c^{trial}, (*a*) 0.6962, the best value in the sense of the method used here; (*b*) 0.701, the maximum value that is allowed by the confidence limits set by Sykes *et al* (1976) using low-density expansions; (*c*) $2^{-1/2}$, the Kondor (1980) conjecture. It is clear that the Kondor conjecture is unlikely to be valid if the assumptions of the present method are accepted. Note that if we vary p_c^{trial} from 0.695 to 0.701, the range found for our estimates of R is 4.5 to 6.0, much larger than the acceptable range.

estimate (8) would have to be multiplied by a factor of 18. Thus we feel that our analysis safely excludes the Kondor value.

We can apply the same approach to site percolation on the square lattice, for which the $n(s, p)$ have been calculated for the matching lattice. The analysis carries through with the same degree of reliability as for the honeycomb lattice, and we find

$$p_c = 0.5923 \pm 0.0007 \qquad \text{(square)}. \tag{8b}$$

Our estimate (9) is safely within the confidence limits of the most accurate previous estimates (Sykes *et al* 1976), $p_c = 0.593 \pm 0.002$, obtained by series expansion methods, and $p_c = 0.5931 \pm 0.0006$, obtained by large-cell Monte Carlo renormalisation group methods (Reynolds *et al* 1980)†.

† We note that our confidence limits are considerably smaller if we further restrict R. Specifically, if we require that values of R for the two matching lattices not only differ by less than 3% but also fall in the range 4.8–5.1, and if we restrict Ω to deviations of not larger than ± 0.05 from the most effective value for a given lattice, then we find (figure 2) $p_c = 0.5923 \pm 0.0004$ (square), and $p_c = 0.6962 \pm 0.0004$ (honeycomb).

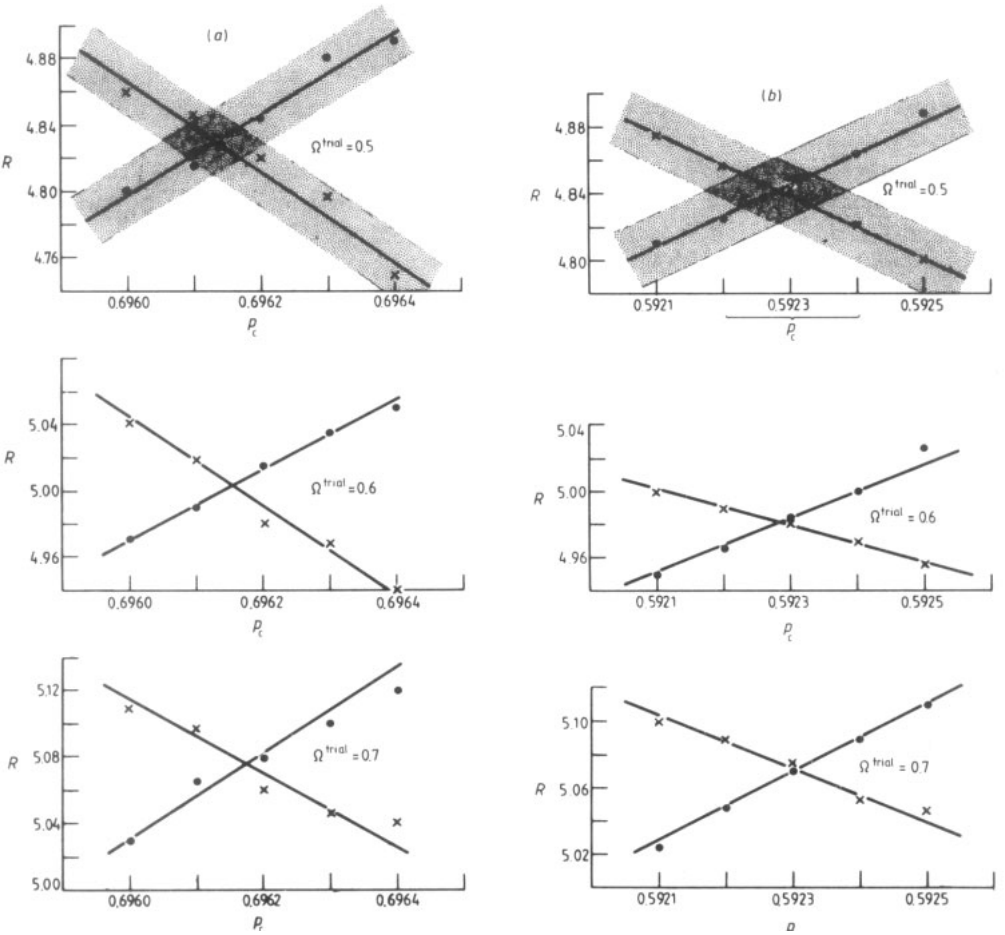

Figure 4. Dependence of R on p_c^{trial} for (a) the honeycomb (HS) and honeycomb match (HMS) lattices, (b) the square (SS) and square match (SMS) lattices. Since the percolation thresholds are related by equation (6), the point of intersection of the two curves shown should represent p_c. Plots are shown for three values of the correction-to-scaling exponent Ω, 0.5, 0.6 and 0.7. Crosses denote the matching lattice, while circles denote the lattice itself.

We checked our methods in the cases TB and HB, which are matching to each other, *and* for which we know p_c exactly. If we analyse the behaviour of R against p_c^{trial} we find that an uncertainty of 3% in R will produce the 'estimates' $p_c = 0.3478 \pm 0.0007$ (TB) and $p_c = 0.6522 \pm 0.0007$ (HB). We see that the exact values of $p_c = 0.3473$ (TB) and $p_c = 0.6527$ (HB) are consistent with our 'estimates'.

In summary, based on the assumed validity of the cluster number scaling hypothesis and the universality of the corresponding scaling function, we have proposed a new method for estimating the percolation threshold p_c. The estimates obtained by this method for most lattices are of roughly the same accuracy as those obtained by conventional series expansion methods, thereby providing an independent check on these other estimates. For the case of the honeycomb and square lattices, the quantities $n(s, p)$ have been calculated for the corresponding matching lattices, and we can use (5) to determine the estimate of p_c *more* accurately than heretofore. We find, in

particular, that for the honeycomb lattice our confidence limits in (8) would have to be multiplied by 18 to include the Kondor conjecture (equation (1)).

After this work was completed, Professors F Y Wu and D Stauffer called our attention to two recent estimates of p_c using quite different methods, both of which support our work. Monte Carlo analysis of the honeycomb lattice (Vicsek and Kertész 1981) suggests $p_c = 0.6973 \pm 0.0008$, which is consistent with (8*a*), and also excludes the Kondor conjecture. Phenomenological renormalisation analysis of the square lattice (Derrida and de Seze 1982) suggests $p_c = 0.5927 \pm 0.0002$, which is also consistent with our estimate (8*b*)†.

We are deeply indebted to M F Sykes for sending us the perimeter polynomials for the honeycomb and square matching lattices prior to their publication (see also Peters *et al* 1979). We also wish to thank I Kondor for having sent us a preprint of his work, and H Nakanishi and D Stauffer for many extremely helpful discussions throughout the course of this work. We thank R K P Zia, F Y Wu, A Coniglio and S Redner for useful comments on various subtle points of the analysis, and A C Brown, E T Gawlinski, H Nakanishi, S Redner, and D Stauffer for reading several drafts of this manuscript.

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† The calculations of Vicsek and Kertesz (1981) and Derrida and de Seze (1982) were concerned each with a single lattice only, while our analysis included 8 lattices. If we had studied only one or two lattices, our confidence limits would have been much tighter since universality would not have restricted us to require such a large range of $R(\pm 3\%)$ to encompass the results of all 8 lattices. For example, suppose we concentrate on a single pair of matching lattices and demand that values of R be the same for two lattices. This means that two numbers should fall within error bars for each of them, which are typically $\pm 0.4\%$ in R. The intersection of the confidence bands for R in figure 4 determines the uncertainty for p_c. For the uncertainty $\pm 0.4\%$ in R, we find $p_c = 0.5923 \pm 0.0001$ (square), and $p_c = 0.6962 \pm 0.0001$ (honeycomb), an accuracy of $\pm 0.02\%$.