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COMMENT

Comment on 'The exact location of partition function zeros, a new method for statistical mechanics'

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Abstract. In a recent paper Wood conjectured that the exact location of the branch point singularity for the hard square lattice gas on the negative activity z axis is at $z = -0.119\,392\ldots$. A careful analysis of the available series data implies that this conjecture is almost certainly false. We find the correct value to be $z = -0.119\,338\,8809 \pm 0.000\,000\,001$, with corresponding exponent indistinguishably close to $\frac{5}{6}$ (corresponding to a zero of the singular part of the function).

Wood (1985) recently proposed a new mathematical technique for the precise location of sections of the locus of the limiting distribution of partition function zeros for model statistical mechanical systems. Motivated by certain properties of the Onsager solution of the two-dimensional Ising model, the conjecture was made for the hard square lattice gas that the branch point singularity of the activity series on the negative real axis is given by the closest negative root of the polynomial

$$2z^6+9z^5+42z^4+90z^3+96z^2+27z+2$$

which yields as the root $z = -0.119\,392\ldots$.

In order to investigate this conjecture, we have used the 42 term low-density series given by Baxter *et al* (1980) for the partition function per site κ as a function of the activity z. The coefficients of this series alternate in sign, suggesting that the dominant singularity is indeed on the negative real axis. Indeed, so dominant is this singularity that Baxter *et al* found no evidence of the physical singularity at $z_c \approx 3.7962$ from this series. In order to determine the nature of the closest singularity, we have utilised seven distinct methods of series analysis. We extrapolated the sequence of ratios, linear extrapolants of successive ratios, unbiased and biased exponent estimates by six sequence extrapolation methods. These were (i) Neville-Aitken extrapolation (Hartree 1952), (ii) the Barber-Hamer algorithm (Barber and Hamer 1982), (iii) Lubkin's three term formula (Lubkin 1952), (iv) Levin's u transform (Levin 1973), (v) the ε transformation (Wynn 1956) and (vi) Brezinski's θ algorithm (Brezinski 1971). We also utilised the method of integral approximants on the original series (Rehr *et al* 1980).

All these methods are described in Guttmann (1987), in which we argue that methods (i) and (vi) are the best sequence extrapolation methods for a wide variety of series in statistical mechanics, with method (iv) being nearly as good, while the

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Table 1. Estimates of the position of the singularity on the negative real axis of the low density $\kappa(z)$ series for the hard square lattice gas, with corresponding exponent extimates.

Method	Estimate of singularity position: From ratio sequence	Estimate of singularity position: From linear extrapolants	Estimate of exponent: Unbiased	Estimate of exponent: Biased ($z = 0.119\,338\,881$)
Neville-Aitken	$\|z\| < 0.119\,339\,6$	$\|z\| > 0.119\,338\,3$	>0.829	$>0.831\,1$
Barber-Hamer	$\|z\| = 0.119\,338\,9$	$\|z\| = 0.119\,338\,9$	$\approx 0.833\,5$	$\approx 0.833\,38$
Lubkin	$\|z\| = 0.119\,338\,8$	—	—	—
Levin u	$\|z\| > 0.119\,338\,1$	$\|z\| \le 0.119\,338\,86$	$\approx 0.833\,7$	$<0.834\,0$
ε algorithm	$\|z\| < 0.119\,92$	$\|z\| < 0.119\,342$	>0.819	$>0.822\,6$
θ transform	$\|z\| = 0.119\,338\,88$	$\|z\| = 0.119\,338\,881$	$\approx 0.833\,37$	$\approx 0.833\,38$

integral approximant method was shown to work well on a wider range of series than the sequence extrapolation algorithms.

In table 1 we show the results of the six sequence extrapolation methods. The implied uncertainty is in the last decimal digit quoted. It can be seen that all six methods are sufficiently precise to rule out Wood's conjecture. Further, they all agree amongst themselves. The most accurate method is Brezinski's θ transform, which gives

$$z^* = -0.119\,338\,8809 \pm 0.000\,000\,001$$

with an (unbiased) exponent estimate of 0.833 37, from which it is an obvious conjecture that the exponent is exactly $\frac{5}{6}$. This means that the low density series behaves like

$$\kappa(z) \sim (z - z^*)^{5/6} \qquad z \to z^*.$$

The method of integral approximants, while less precise than the best of the sequence extrapolation methods, gives the estimates $z^* = -0.119\,3390$, with exponent estimates greater than 0.831. Thus all seven methods are consistent, and all rule out the conjecture. It is interesting to note that Gaunt and Fisher (1965) were the first to consider this exponent, and noted that it was 'approximately 0.8'.

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