Dimer λ_d Expansion Computer Computations

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Abstract

In a previous paper an asymptotic expansion for λ_d in powers of $1/d$ was developed. The results of computer computations for some terms in the expansion, as well as various quantities associated to the expansion, are herein presented. The computations (in integer arithmetic) are actually done only for $d = 1, d = 2$, and $d = 3$, but some results for arbitrary dimension follow from the general structure of the theory. In particular we obtain the next term in powers of $1/d$, the $1/d^3$ term in the asymptotic expansion for λ_d, as well as checking the correctness of the terms previously calculated by hand.

For $d = 2$ and $d = 3$ a second expansion for λ_d is defined and numerically studied. Contrary to our hopes this second type of expansion appears not to be convergent. There is not enough evidence to argue if the expansions for λ_d in powers of $1/d$ are convergent for either $d = 2$ or $d = 3$, but likely they are not. (Certainly convergence, but at a very slow rate, remains an interesting possibility in all our cases.)

In [1] an expansion for λ_d in powers of $1/d$ was presented, completing the asymptotic expression obtained in [2], by Minc. The expression as presented in [1] is

$$\lambda_d \sim \frac{1}{2}\, ln(2d) - \frac{1}{2} + \frac{1}{8}\frac{1}{d} + \frac{5}{96}\,\frac{1}{d^2} + \,\cdots \tag{1}$$

One result of this paper is the extension for one more power of $1/d$

$$\lambda_d \sim \frac{1}{2}\, ln(2d) - \frac{1}{2} + \frac{1}{8}\frac{1}{d} + \frac{5}{96}\,\frac{1}{d^2} + \frac{5}{64}\,\frac{1}{d^3} + \cdots . \tag{2}$$

The key quantities to be computed are the $\bar{J}_i$ defined in equation (28) of [1], and the note after (33) therein

$$\bar{J}_i = \frac{1}{N}\,\frac{1}{i!}\,J_i \tag{3}$$

The first few $\bar{J}_i$ are given in (29) and (38) of [1].

We have used Maple software to compute the $\bar{J}_i$ for $i = 1,2,3,4,5,6;\ d = 1,2,3$ as given in the following.

<u>For $d = 1$ one has</u>:

$$\bar{J}_1 = 0 \tag{4}$$
$$\bar{J}_2 = 1/8 \tag{5}$$
$$\bar{J}_3 = 1/12 \tag{6}$$
$$\bar{J}_4 = -\,3/64 \tag{7}$$
$$\bar{J}_5 = -\,13/80 \tag{8}$$
$$\bar{J}_6 = -\,19/192 \tag{9}$$

<u>For $d = 2$ one has:</u>

$$\bar{J}_1 = 0 \tag{10}$$
$$\bar{J}_2 = 1/16 \tag{11}$$
$$\bar{J}_3 = 1/48 \tag{12}$$
$$\bar{J}_4 = -\,9/512 \tag{13}$$
$$\bar{J}_5 = -\,23/1280 \tag{14}$$
$$\bar{J}_6 = 25/3072 \tag{15}$$

For $d = 3$ one has:

$$\begin{aligned}
\bar{J}_1 &= 0 && (16)\\
\bar{J}_2 &= 1/24 && (17)\\
\bar{J}_3 &= 1/108 && (18)\\
\bar{J}_4 &= -\,5/576 && (19)\\
\bar{J}_5 &= -\,11/2160 && (20)\\
\bar{J}_6 &= 175/46656 && (21)
\end{aligned}$$

The results above for $\bar{J}_i$, $i \leq 4$, were presented in [1] as obtained by hand computation.

The $\bar{J}_i$ for $d = 1$ are computable in seconds of computer time, and $\bar{J}_i$ with much higher values of i are easily obtained. For $d = 2$ and $d = 3$ the $\bar{J}_6$ required several days of computer time; $\bar{J}_7$ would be extremely difficult to obtain, requiring both more theory and much more computer time, a year's effort.

The results, (4) through (21), and equation (30) of [1] (whose proof will appear in a later paper), will establish the following formulae for $\bar{J}_i$ in general dimension:

$$\begin{aligned}
\bar{J}_1 &= 0 && (22)\\
\bar{J}_2 &= \frac{1}{8}\,\frac{1}{d} && (23)\\
\bar{J}_3 &= \frac{1}{12}\,\frac{1}{d^2} && (24)\\
\bar{J}_4 &= -\,\frac{3}{32}\,\frac{1}{d^2} + \frac{3}{64}\,\frac{1}{d^3} && (25)\\
\bar{J}_5 &= -\,\frac{1}{8}\,\frac{1}{d^3} - \frac{3}{80}\,\frac{1}{d^4} && (26)\\
\bar{J}_6 &= \frac{7}{48}\frac{1}{d^3} - \frac{5}{64}\frac{1}{d^4} - \frac{1}{6}\frac{1}{d^5} && (27)
\end{aligned}$$

Substituting these values of $\bar{J}_i$ into (36) of [1], and extracting the behavior of the exponent in (36) to order $1/d^3$, we get the result in (2) above. We are using the fact that $\bar{J}_i$ for $i > 6$ have only powers of $1/d$ greater than 3.

For $d = 2$ and $d = 3$ we have considered two sequences of approximations each characterized by keeping more and more terms in some sense. The first sequence of approximations

$$A_0, A_1, \cdots \tag{28}$$

is constructed from

$$\lambda_d \sim \frac{1}{2}\, ln(2d) - \frac{1}{2} + \frac{c_1}{d} + \frac{c_2}{d^2} + \cdots \tag{29}$$

by

$$A_r = \frac{1}{2}\, ln(2d) - \frac{1}{2} + \sum_{i=1}^{r} \frac{c_i}{d^i}. \tag{30}$$

We then have the results:

<u>For $d = 2$</u>:

$$A_0 = .1931 \tag{31}$$
$$A_1 = .2556 \tag{32}$$
$$A_2 = .2687 \tag{33}$$
$$A_3 = .2784 \tag{34}$$

Of course here, for $d = 2$, the exact result $\lambda_2 = .29156....$ is known. [3], [4]

<u>For $d = 3$</u>:

$$A_0 = .3959 \tag{35}$$
$$A_1 = .4375 \tag{36}$$
$$A_2 = .4433 \tag{37}$$
$$A_3 = .4462 \tag{38}$$

Exact bounds for λ_3 as given in [5] are

$$.440075 \leq \lambda_3 \leq .457547 \tag{39}$$

Our second sequence of approximations is

$$B_0, B_1, \cdots \tag{40}$$

constructed by replacing $\bar{J}_i$ by $\bar{J}_i\ x^{i-1}$ with x a formal parameter. We then substitute these $\bar{J}_i\ x^{i-1}$ for $\bar{J}_i$ in (36) of [1]. To obtain B_r, keeping terms through power x^r (and then setting $x = 1$), we get the values:

<u>for d = 2</u>:

$$B_0 = .1931 \tag{41}$$
$$B_1 = .2556 \tag{42}$$
$$B_2 = .2921 \tag{43}$$
$$B_3 = .2992 \tag{44}$$
$$B_4 = .2905 \tag{45}$$
$$B_5 = .2814 \tag{46}$$

<u>and for d = 3</u>:

$$B_0 = .3959 \tag{47}$$
$$B_1 = .4375 \tag{48}$$
$$B_2 = .4538 \tag{49}$$
$$B_3 = .4524 \tag{50}$$
$$B_4 = .4468 \tag{51}$$
$$B_5 = .4445 \tag{52}$$

Originally we hoped the sequence of B_i converged, but this now seems unlikely. If the sequences of B_i for $d = 2$ and $d = 3$ behaved similarly, we might have an argument that $\lambda_3 = .453 \pm .001$. We do not know whether to believe this or not.

It remains to outline the general flow of the computer computations. The quantities of interest were obtained through a chain of operations successively performed. Were we to redo the hand calculation of $\bar{J}_4$ as described in [1], we would find it much more efficient to echo some of the ideas used in the computer programs. Naturally we cannot describe the many little clever ideas, saving memory and increasing efficiency, needed to push the computations to the level of obtaining $\bar{J}_6$. We find it convenient to describe our computations as divided into four steps, which we present in inverse order.

Step 4. This step assumes knowledge of the $\bar{J}_i$, and substitutes them into (36) of [1] to obtain the approximations A_i and B_i.

Step 3. This step assumes known the quantities

$$\sum_{s_1,s_2,\ldots,s_s} f(\bar{s}_1)\cdots f(\bar{s}_s)\psi_c'(s_1,s_2,\ldots,s_s) \tag{53}$$

(where f is as in [1], $\frac{1}{2d}$ on a dimer, zero on other tiles, and (53) is as (28) of [1] with v replaced by f) and computes

$$J_s = \sum_{s_1,s_2,\ldots,s_s} v(\bar{s}_1)\cdots v(\bar{s}_s)\psi_c'(s_1,s_2,\ldots,s_s). \tag{54}$$

Step 2. Takes the output of Step 1 described next to yield the expression in equation (53) above.

Note that in equations (53) and (54) above the sums are over all located tiles $s_1,\ldots,s_s$ such that the sequence is connected. That is, one cannot pick two subsets of ordered sets $s_1,\ldots,s_s$ such that, with the two sub-ordered sequences

$$s_{\alpha_1}\ ,\ldots,\ s_{\alpha_r}\quad\text{and}\quad s_{\beta_1}\ ,\ldots,\ s_{\beta_r}$$

one has

1) the same s_i appear in $s_1,\ldots,s_s$ and in the union of the two sub-ordered sets, with the same multiplicity
2) the two sub-ordered sets of located tiles have no overlap between them.

We now define an s-*dimer tree* to be an ordered sequence of s located tiles $s_1,s_2,\ldots,s_s$ such that for each $i\leq s$ the sequence of located tiles $s_1,s_2,\ldots,s_i$ is connected. It is easy to see s-*dimer trees* are the sort of thing a computer can easily generate.

Step 1. The output of Step 1 (towards computation of J_s) is the set of all possible *s-dimer trees* with given s_1. With each *s-dimer tree* the output of Step 1 also includes knowledge of the overlap pattern of the tree. That is, for the tree $s_1, ..., s_s$ one knows whether $s_i \cap s_j$ is empty or not for each i and j. (The output of Step 1 actually yields the number of *s-dimer trees* with each overlap pattern.)

Steps 3 and 4 take seconds to run in the cases we have studied. In the computation of $\bar{J}_6$, Step 1 and Step 2 required several weeks of computer time.

References

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