For the Monomer-Dimer $\lambda_d(p)$, the Master Algebraic Conjecture

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Abstract

The author has recently presented two different expressions for $\lambda_d(p)$ of the monomer-dimer problem involving a power series in p, the first jointly with Shmuel Friedland. These two expressions are certainly equal, but this has not yet been proven rigorously. The first is naturally developed from quantities $\bar{J}_i$, cluster expansion kernels. The second from the Mayer (or Virial) series of a dimer gas, in particular from the b_i coefficients in the Mayer series. The sets $\{b_i\}$ and $\{\bar{J}_i\}$ can be derived from each other. Given an arbitrary set of values for either the b_i or the $\bar{J}_i$ both expressions may be given in terms of a formal sum. The master algebraic conjecture is that these two expressions are equivalent. This is detailed in the special case all $\bar{J}_i$ are zero.

1 Introduction

Shmuel Friedland and the author recently presented an expression for $\lambda_d(p)$ of the monomer-dimer problem involving a power series in p, see eq (7.1) of [1]. I have proven the series converges for small enough p, [2]. More recently I found another similar expression for $\lambda_d(p)$ related in a suitable sense to the Mayer (or Virial) expansion of the dimer gas, [3]. It is known that this series converges for small enough p, [4]. The two series are certainly equivalent, but this has not yet been proven. It should be straight forward to prove the second expression converges to the correct value. The then two equivalent and seemingly very difficult tasks are either proving the two expressions for $\lambda_d(p)$ are equivalent, or proving the first series converges to the correct value. It may first strike one that one should only work with the second expression, as being easier to construct proofs for, but it is the first expression with its development which incorporates the details of dependence on the dimension. We herein generalize the problem of the equivalence between the two expressions. We specify arbitrary values for the set of $\bar{J}_i$ (or equivalently the set of b_i) and then construct each of the two expressions ... for $\lambda_d(p)$ if the values were correctly picked ... now each involving formal power series. (Whenever there is question all expressions in the paper are taken as formal expansions about zero in all variables.) The Master Conjecture is that the two expressions are equivalent, the formal sums are equivalent. To the author this result has some of the magical beauty that devotees of string theory sometimes see in their cult teachings. Section 2 displays the transition from the $\{b_i\}$ to the$\{\bar{J}_i\}$ and visa-versa. Section 3 constructs the first expansion, and Section 4 the second expansion. Section 5 discusses the case when all $\bar{J}_i$ are zero.

2 From $\{b_i\}$ to$\{\bar{J}_i\}$ and Visa-Versa

We present the formulae we have used to derive the $\bar{J}_i$ from the b_i in all our previous work, though they were not explicitly written down. They were implicitly mentioned in [5].(See the remark there in the paragraph following the paragraph containing eq. (30), the sentence beginning: "By a simple device...".) They follow upon consideration of the relation between the cluster expansion kernels developed with interaction ν and that with interaction f as both considered in [5]. We will always impose the conditions

$$b_1 = d \tag{1}$$

and

$$\bar{J}_1 = 0. \tag{2}$$

The $\bar{J}_r$ are inductively determined from $r = 2$ on by

$$\bar{J}_r = \lim_{L\to\infty} \frac{1}{L} \left\{ S_r - (\exp(L\sum_{i=0}^{r-1} \bar{J}_i x^i))|_r \right\}. \tag{3}$$

where

$$S_r = \sum_{p=0}^{r} \left\{ (exp(L\sum_i b_i(\frac{x}{2d})^i))|_p \frac{1}{(r-p)!} \left(\frac{-1}{2(L-1)}\right)^{r-p} \frac{(L-2p)!}{(L-2r)!} \right\}. \tag{4}$$

The symbol $|$ with the subscript j indicates the jth coefficient in the formal power series in x. It is easy to see that we may also inductively go from the $\bar{J}_i$ to the b_i by the same formulae. We present now the explicit formulae thus obtained for the first six terms going in each direction. We will several times give the first six terms explicitly for quantities to help the reader see relevant patterns, to suggest things they might want to prove.

$$\bar{J}_2 = -\frac{1}{4}\frac{1}{d^2}(-2d^2 - b_2) \tag{5}$$

$$\bar{J}_3 = \frac{1}{24}\frac{1}{d^3}(3b_3 + 24db_2 + 28d^3) \tag{6}$$

$$\bar{J}_4 = -\frac{1}{16}\frac{1}{d^4}(-12db_3 - 28d^4 - b_4 - 40d^2b_2) \tag{7}$$

$$\bar{J}_5 = \frac{1}{160}\frac{1}{d^5}(5b_5 + 480d^3b_2 + 48d^5 - 80db_2^2 + 420d^2b_3 + 80db_4) \tag{8}$$

$$\bar{J}_6 = -\frac{1}{192}\frac{1}{d^6}(-1056d^3b_3 + 1584d^4b_2 - 432d^2b_4 + 1760d^6 - 3b_6 + 144db_3b_2 + 1056d^2b_2^2 - 60db_5) \tag{9}$$

$$b_2 = d^2(4\bar{J}_2 - 2) \tag{10}$$

$$b_3 = \frac{4}{3}d^3(5 - 24\bar{J}_2 + 6\bar{J}_3) \tag{11}$$

$$b_4 = 2d^4(-14 + 8\bar{J}_4 + 112\bar{J}_2 - 48\bar{J}_3) \tag{12}$$

$$b_5 = \frac{16}{5}d^5(42 + 10\bar{J}_5 - 480\bar{J}_2 - 80\bar{J}_4 + 270\bar{J}_3 + 80\bar{J}_2^2) \tag{13}$$

$$b_6 = \frac{16}{3}d^6(-132 - 120\bar{J}_5 + 1980\bar{J}_2 + 528\bar{J}_4 - 1320\bar{J}_3 - 1056\bar{J}_2^2 + 12\bar{J}_6 + 288\bar{J}_3\bar{J}_2) \tag{14}$$

3 The First Expression for $\lambda_d(p)$

Shmuel Friedland and the author presented the 'first expression' for $\lambda_d(p)$ in [1]. We here write it in the form

$$\lambda_d(p) = Q_1 + Q_2 \tag{15}$$

$$Q_1 = \frac{1}{2}\left(p\ln(2d) - p\ln p - 2(1-p)\ln(1-p) - p\right) \tag{16}$$

$$Q_2 = \sum_{k=2} a_k p^k. \tag{17}$$

We take our construction of the a_i from [2]. First as in earlier work we define the α_i. One solves the following equation by iteration from $\alpha_i = 0$.

$$\alpha_k = \left(\bar{J}_k p^k\right) \cdot \frac{1}{(1 - 2\sum i\alpha_i)^{2k}} \cdot \left(1 - 2\sum i\alpha_i/p\right)^k \tag{18}$$

Then Q_2 is given as

$$Q_2 = \sum \alpha_i - \sum_{k=2}\frac{1}{k}\left(2\sum_i i\alpha_i\right)^k + \frac{1}{2}p\sum_{k=2}\frac{1}{k}\left(2\sum_i i\alpha_i/p\right)^k. \tag{19}$$

We now list the values of the first few a_i, as derived from equations (17) - (19).

$$a_2 = \bar{J}_2 \tag{20}$$

$$a_3 = -4\bar{J}_2^2 + \bar{J}_3 \tag{21}$$

$$a_4 = \bar{J}_4 - 12\bar{J}_2\bar{J}_3 + \frac{80}{3}\bar{J}_2^3 + 8\bar{J}_2^2 \tag{22}$$

$$a_5 = -128\bar{J}_2^3 + \bar{J}_5 + 24\bar{J}_2\bar{J}_3 - 16\bar{J}_2\bar{J}_4 - 9\bar{J}_3^2 - 224\bar{J}_2^4 + 144\bar{J}_2^2\bar{J}_3 \tag{23}$$

$$\begin{aligned} a_6 = \frac{416}{3}\bar{J}_2^3 + 32\bar{J}_2\bar{J}_4 + \frac{10752}{5}\bar{J}_2^5 + 18\bar{J}_3^2 \\ +1792\bar{J}_2^4 + 224\bar{J}_4\bar{J}_2^2 + 252\bar{J}_3^2\bar{J}_2 \\ -1792\bar{J}_2^3\bar{J}_3 + \bar{J}_6 - 672\bar{J}_2^2\bar{J}_3 - 24\bar{J}_3\bar{J}_4 - 20\bar{J}_2\bar{J}_5 \end{aligned} \tag{24}$$

4 The Second Expression for $\lambda_d(p)$

We follow the development of the 'second expression' in [3], in which this relation for $\lambda_d(p)$ was first introduced. (We there modestly cleped this expression 'the Federbush relation'.) One started with the Mayer series.(We will set $\beta = 1$).

$$\beta P = \sum_{n=1}^{\infty} b_n z^n \tag{25}$$

and the relation for p thought of as twice the density of dimers

$$p = 2\sum_{1}^{\infty} n b_n z^n. \tag{26}$$

or

$$z = \frac{1}{2b_1}p - \sum_{2}^{\infty} \frac{n b_n}{b_1} z^n.$$

We solved this for $z = z(p)$ iterating from $z = 0$. Substituting this into the right side of eq.(25), one gets

$$P(p) = \sum_{1}^{\infty} b_n (z(p))^n \tag{27}$$

Written as a power series in p this is the Virial series. We write $z(p)$ as

$$z = \frac{p}{2b_1}(1 + F(p)). \tag{28}$$

Using the same notation as in eq. (15) and (16), the 'second expression' has for Q_2 the relation

$$Q_2 = \frac{1}{2}\left(2(1-p)\ln(1-p) + p\right) + P(p) - \frac{p}{2}\ln(1 + F(p)). \tag{29}$$

We now list the expressions derived for the first few a_i explicitly

$$a_2 = \frac{1}{4}\frac{1}{d^2}(2d^2 + b_2) \tag{30}$$

$$a_3 = -\frac{1}{24}\frac{1}{d^4}(-4d^4 - 3b_3 d + 6b_2^2) \tag{31}$$

$$a_4 = \frac{1}{48}\frac{1}{d^6}(4d^6 - 18b_3 b_2 d + 20b_2^3 + 3b_4 d^2) \tag{32}$$

$$a_5 = -\frac{1}{320}\frac{1}{d^8}(-10d^3 b_5 + 45d^2 b_3^2 - 360b_2^2 d b_3 + 80d^2 b_4 b_2 + 280b_2^4 - 16d^8) \tag{33}$$

$$a_6 = \frac{1}{960}\frac{1}{d^{10}}(2016b_2^5 - 180b_3 d^3 b_4 + 840d^2 b_4 b_2^2 + 32d^{10}$$
$$+945b_3^2 d^2 b2 + 15b_6 d^4 - 150b_5 b_2 d^3 - 3360b_3 d b_2^3) \tag{34}$$

5 Special case, all $\bar{J}_i = 0$

We first define $\tilde{b}_n$

$$\tilde{b}_n = \frac{1}{n}(-1)(-1)^n d^n 2^{n-1} C_n \tag{35}$$

where C_n is the Catalan number

$$C_n = \frac{(2n)!}{(n+1)!n!} \tag{36}$$

Conjectured Theorem, The set of $\bar{J}_i$ with all $\bar{J}_i = 0$ corresponds to the set of b_i with all $b_i = \tilde{b}_i$ under the transformations in Section 2. Both of the expressions for $\lambda_d(p)$ yield $Q_2 = 0$ in this case.

We break the proof into three parts, but we can prove only the first two parts.

1) If all $\bar{J}_i = 0$ expression one gives $Q_2 = 0$.
2) If all $b_i = \tilde{b}_i$ then expression two gives $Q_2 = 0$.
3) The set of all $\bar{J}_i = 0$ corresponds to the set of all $b_i = \tilde{b}_i$.

We note that the truth of 1) is a trivial observation.

We turn to the proof of 2), basically a number of computations. We write down the well known generating function for the Catalan numbers

$$\sum_{n=0}^{\infty} C_n x^n = \frac{1-(1-4x)^{1/2}}{2x} = \frac{2}{1+(1-4x)^{1/2}} \tag{37}$$

If we substitute $\tilde{b}_n$ for b_n into eq. (26) we get

$$p = 1 - \sum_{0}^{\infty} (-2dz)^n C_n \tag{38}$$

We set $x = -2dz$ and then eq. (38) becomes

$$1 - p = \frac{1 - (1 - 4x)^{1/2}}{2x} \tag{39}$$

or

$$x = -\frac{p}{(1-p)^2} \tag{40}$$

which becomes

$$z = \frac{p}{2d(1-p)^2} \tag{41}$$

We substitute this into eq. (27) to get

$$P(p) = -\frac{1}{2} \sum_{1}^{\infty} \frac{1}{n} \left(\frac{-p}{(1-p)^2} \right)^n C_n \tag{42}$$

A little calculation using the generating function leads to

$$P = -\frac{p}{2} - \ln(1-p) \tag{43}$$

From eq. (28) and eq. (41) we directly get

$$1 + F = \frac{1}{(1-p)^2} \tag{44}$$

We now substitute eq. (43) and eq. (44) into eq. (29) and we get the desired result

$$Q_2 = 0. \tag{45}$$

The final task is to prove 3) above. We do not now know how to do this, but we write down what must be shown. We first find the expression for the sum in the exponential of eq. (4)

$$e(x) \equiv \sum_i \tilde{b}_i (\frac{x}{2d})^i = \frac{1}{1 + (1+4x)^{1/2}} + \ln(1 + (1+4x)^{1/2}) - \frac{1}{2} - \ln(2) \tag{46}$$

by a similar computation to that for eq. (43). Now what one has to prove is

$$0 = \lim_{L \to \infty} \frac{1}{L} \left\{ \sum_{p=0}^{r} (exp(Le(x)))|_p \frac{1}{(r-p)!} \left(\frac{-1}{2(L-1)} \right)^{r-p} \frac{(L-2p)!}{(L-2r)!} \right\} \tag{47}$$

where the bar with subscript has the same meaning as in eq. (3) and eq. (4).

Hopefully someone perhaps a little smarter than me, and certainly a lot younger, will prove this...and even the full master algebraic conjecture.

References

[1] P. Federbush and S. Friedland, "An Asymptotic Expansion and Recursive Inequalities for the Monomer-Dimer Problem," *Jour. of Stat. Phys* 143 (2011), 306.

[2] P. Federbush, "Convergence of the Formal Expansion for $\lambda_d(p)$ of the Monomer-Dimer Problem for Small p," arXiv:1101.4591.

[3] P. Federbush, "The Dimer Gas Mayer Series, the Monomer-Dimer $\lambda_d(p)$, the Federbush Relation," arXiv:1207.1252.

[4] Ruelle, David, *Statistical Mechanics*, W. A. Benjamin, Inc. Amsterdam, 1969

[5] P. Federbush, "Computation of Terms in the Asymptotic Expansion of Dimer λ_d for High Dimensions," *Phys. Lett. A* 374 (2009), 131-133.