Convergence of the Formal Expansion for $\lambda_d(p)$ of the Monomer-Dimer Problem for Small p

Paul Federbush
Department of Mathematics
University of Michigan
Ann Arbor, MI 48109-1043
(pfed@umich.edu)

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Abstract

Shmuel Friedland and the author recently presented a formal expansion for $\lambda_d(p)$ of the monomer-dimer problem. Herein we prove that if the terms in the expansion are rearranged as a power series in p, then for sufficiently small p this series converges.

In a series of papers the author presented a formal asymptotic expansion for λ_d of the dimer problem, in inverse powers of d. See [1]. The expansion is as follows

$$\lambda_d \sim \frac{1}{2}\ln(2d) - \frac{1}{2} + \sum_{k=1} \frac{c_k}{d^k} \tag{1}$$

computed through the $k = 3$ term as

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

In a recent paper, [2], Shmuel Friedland and the author extended this work to yield a formal asymptotic expansion for $\lambda_d(p)$ of the dimer-monomer problem

$$\lambda_d(p) \sim \frac{1}{2}\left(p\ln(2d) - p\ln p - 2(1-p)\ln(1-p) - p\right) + \sum_{k=1} \frac{c_k(p)}{d^k} \tag{3}$$

computed through the $k = 3$ term as

$$\begin{aligned}\lambda_d(p) \sim &\frac{1}{2}\left(p\ln(2d) - p\ln p - 2(1-p)\ln(1-p) - p\right)\\ &+ \frac{1}{8}\frac{p^2}{d} + \frac{\left(2p^3 + 3p^4\right)}{96}\frac{1}{d^2} + \frac{\left(-5p^4 + 12p^5 + 8p^6\right)}{192}\frac{1}{d^3}.\end{aligned} \tag{4}$$

For given d we rearrange the expansion in (3) as a power series in p

$$\lambda_d(p) \sim \frac{1}{2}\left(p\ln(2d) - p\ln p - 2(1-p)\ln(1-p) - p\right) + \sum_{k=2} a_{d,k}p^k. \qquad (5)$$

We see from (4) that

$$a_{d,2} = \frac{1}{8}\frac{1}{d} \qquad (6)$$

$$a_{d,3} = \frac{1}{48}\frac{1}{d^2} \qquad (7)$$

$$a_{d,4} = \frac{1}{32}\frac{1}{d^2} - \frac{5}{192}\frac{1}{d^3}. \qquad (8)$$

We have here used the fact that $C_k(p)$ of equation (3) is a sum of powers p^s where $k < s \leq 2k$, see Lemma 4 and Theorem 2 below. It is the primary goal of this paper to show that if p is small enough ($0 \leq p < p_0$, p_0 independent of d) the sum in (5) converges, see Theorem 4 below. (Throughout the paper we are not careful about getting the best value of p_0; with any improvements we could make to the current procedure the value we get for p_0 would still be anemic.)

We will assume familiarity with Section 5 of [2], and use many of the formulae therefrom. $\lambda_d(p)$ is determined, by a complicated computation, from the infinite sequence of cluster expansion kernels

$$\bar{J}_1, \bar{J}_2, \bar{J}_3, \ldots \qquad (9)$$

defined in equations (5.21), (5.23). (We will not indicate herein that such (5.–) equation comes from [2].) The first six $\bar{J}_i$ have been computed and are listed in (5.25) – (5.30). From (5.17) and (5.31) an infinite sequence of auxiliary quantities

$$\alpha_1, \alpha_2, \ldots \qquad (10)$$

are computed from the $\bar{J}_i$. An easy computation from (5.17) and (5.31) leads to the nice expression

$$\alpha_k = \left(\bar{J}_k p^k\right) \cdot \frac{1}{\left(1 - 2\sum i\alpha_i\right)^{2k}} \cdot \left(1 - 2\sum i\alpha_i/p\right)^k \qquad (11)$$

which replaces (5.31).

We view the α_k as determined from (11) by recursive iteration. Later working with bounds on the $\bar{J}_k$ we will study values of p for which iterations converge to a *solution* of (11).

From (5.10), (5.11), and (5.12) we have that

$$\lambda_d(p) = S + \lim_{N\to\infty} \frac{1}{N} \ln Z^* \qquad (12)$$

where we have defined

$$S \equiv \frac{p}{2}\ln(2d) - \frac{p}{2}\ln p - (1-p)\ln(1-p) - \frac{p}{2}. \tag{13}$$

Now from (5.32), (5.31), and (5.17) we may easily compute

$$\lambda_d(p) = S + \sum \alpha_i - \sum_{k=2} \frac{1}{k}\left(2\sum_i i\alpha_i\right)^k + \frac{1}{2}p\sum_{k=2}\frac{1}{k}\left(2\sum_i i\alpha_i/p\right)^k. \tag{14}$$

Equations (11), (13), and (14) are our master equations. All our results below concern solutions of these equations, we do not address here whether such solutions actually correspond to a computation of the monomer-dimer partition function as

$$\sum \text{covers} \sim e^{N\lambda_d(p)} \tag{15}$$

although certainly this is the case.

We state the information in equation (5.22) as a lemma.

Lemma 1. *$\bar{J}_k$ is a sum of inverse powers of d, $(1/d)^s$, with*

$$\frac{k}{2} \leq s < k \tag{16}$$

Lemma 2. *At the first iteration of equation (11) α_k is a sum of powers of p and $(1/d)$, $p^i\,(1/d)^j$, with*

$$\begin{gathered} i = k \\ \frac{i}{2} \leq j < i \end{gathered} \tag{17}$$

Lemma 3. *At the end of any number of iterations of equation (11) α_k is a sum of terms $p^i\,(1/d)^j$ with*

$$\begin{gathered} i \geq k \\ \frac{i}{2} \leq j < i \end{gathered} \tag{18}$$

Lemma 4. *Substituting the α_k as satisfying (18) into (14) one finds $\lambda_d(p) - S$ is a sum of terms $p^i\,(1/d)^j$ satisfying (18).*

These lemmas are easily proven by studying the evolution of powers of p and $(1/d)$ through the iterations and expansions.

One may consider the formal expansion of α_k after an infinite number of iterations of (11), and its substitution into (14), yielding an infinite formal expansion for $\lambda_d(p) - S$. These also are a sum of terms $p^i\,(1/d)^j$ satisfying (18).

We reorganize our formal expansions as a power series in p.

$$\alpha_k = \sum_{s=k} p^s f_{k,s} \tag{19}$$

$$\lambda_d(p) = S + \sum_{s=2} p^s g_s \tag{20}$$

The $f_{k,s}$ and g_s are built up of powers of $(1/d)$, $(1/d)^i$ satisfying

$$\frac{s}{2} \leq i < s \tag{21}$$

We now consider working with a fixed value of d, and assume we have a bound on the $\bar{J}_k$

$$|\bar{J}_k| \leq B^k, \quad k = 1, 2, \ldots \tag{22}$$

for some B. Under these circumstances we set up the machinery to use the contraction mapping principle. On any formal infinite polynomial in p

$$f = \sum a_i p^i \tag{23}$$

we define a norm $|f|$

$$|f| \equiv \sum |a_i p^i|. \tag{24}$$

This norm has the properties

$$P1) \qquad |cf| = |c||f| \tag{25}$$

$$P2) \qquad |f + g| \leq |f| + |g| \tag{26}$$

$$P3) \qquad |fg| \leq |f||g| \tag{27}$$

for scalar c and polynomials f and g.

We denote the sequence of α_k, as in (10), by α, and define a norm on α

$$\|\alpha\| = \sum_k 2^k |\alpha_k|. \tag{28}$$

We find an ε, $0 < \varepsilon < 1/2$, small enough so that

$$\frac{1}{2} \frac{1}{(1 - 2\varepsilon)^2} (1 + 2\varepsilon) \leq 1 \tag{29}$$

and

$$\frac{6\varepsilon}{1 - 2\varepsilon} \leq 1. \tag{30}$$

We then require $p > 0$ to be small enough that

$$p^{k-1} B^k \leq \varepsilon \frac{1}{8^k}, \quad k = 2, 3, \ldots \tag{31}$$

Working with this choice of ε and p we define the complete metric space $\mathcal{S}$ on which we establish a contraction mapping

$$\mathcal{S} = \{\alpha = \{\alpha_k\} \mid \|\alpha\| \le p\varepsilon\} \tag{32}$$

We rewrite (11) as

$$\alpha_k = f_k(\alpha), \quad k = 2, 3, \dots \tag{33}$$

or

$$\alpha = f(\alpha). \tag{34}$$

Conditions (29) and (31) ensure that f carries $\mathcal{S}$ into $\mathcal{S}$. With the further condition (30) one establishes that f is a contraction.

Theorem 1. *With the conditions on p and ε above, there is a unique solution of* (34) *in $\mathcal{S}$, exactly the one obtained by iteration of* (11).

Substituting this solution into (14) one obtains the expression for $\lambda_d(p)$. We collect the properties of this quantity.

Theorem 2. *For $0 < p \le p_0$, p_0 determined by* (31),

$$\lambda_d(p) = \frac{p}{2}\ln(2d) - \frac{p}{2}\ln p - (1-p)\ln(1-p) - \frac{p}{2} + \sum_{s=2} p^s g_s \tag{35}$$

where g_s is a polynomial in $(1/d)$ with powers $(1/d)^i$ satisfying

$$\frac{s}{2} \le i < s. \tag{36}$$

The sum in (35) *is absolutely convergent. g_s is a polynomial in $\bar{J}_1, \bar{J}_2, \dots, \bar{J}_s$ and is determined by a finite number of iterations of* (11) *substituted into* (14). *One need only keep the finite number of terms throughout whose power of p is less than or equal to s to get g_s.*

We content ourselves with presenting the proof that the f of (34) maps $\mathcal{S}$ into $\mathcal{S}$. We look at the mapping of (33) carrying α_k into α'_k

$$\alpha'_k = f_k(\alpha) \tag{37}$$

and we wish to prove if α is in $\mathcal{S}$ then α' is in $\mathcal{S}$. Parallel to (11) we have

$$\alpha'_k = \left(\bar{J}_k p^k\right) \cdot \frac{1}{\left(1 - 2\sum i\alpha_i\right)^{2k}} \left(1 - 2\sum i\alpha_i/p\right)^k. \tag{38}$$

We take the $|\cdot|$ norm of both sides using *P1, P2, P3* of (25)–(27).

By (31), (22), and (28),

$$|\alpha_k'| \le p\varepsilon \frac{1}{8^k} \left(\frac{1}{1 - 2\sum i|\alpha_i|} \right)^{2k} \left(1 + 2\sum i|\alpha_i|/p \right)^k \tag{39}$$

$$\le p\varepsilon \frac{1}{2^k} \left(\frac{1}{(1-2\|\alpha\|)^2} \cdot \frac{(1+2\|\alpha\|/p)}{2} \right)^k \frac{1}{2^k} \tag{40}$$

and since $\alpha \in \mathcal{S}$

$$\le p\varepsilon \frac{1}{2^k} \left(\frac{1}{(1-2\varepsilon p)^2} \frac{(1+2\varepsilon)}{2} \right)^k \frac{1}{2^k} \tag{41}$$

using (29)

$$\le p\varepsilon \frac{1}{2^k} \frac{1}{2^k}. \tag{42}$$

Or

$$2^k |\alpha_k'| \le p\varepsilon \frac{1}{2^k} \tag{43}$$

so that

$$\|\alpha'\| = \sum_2 2^k |\alpha_k'| \le p\varepsilon \sum_2 \frac{1}{2^k} \le p\varepsilon \frac{1}{2} \tag{44}$$

and thus $\alpha' \in \mathcal{S}$ as was to be proved.

Theorem 3. *There is a value of B_0 that ensures*

$$|\bar{J}_n| \le B_0^n, \quad n = 1, 2, \ldots$$

for all values of d.

Theorem 4. *There is a value p_0 (independent of d) such that for $0 \le p < p_0$ the series for $\lambda_d(p)$ in (5) converges.*

Theorem 4 follows from Theorem 3 by the development above.

We turn to Theorem 3. In fact we will see $B_0 = 8e$ works. We could follow the general cluster expansion formalism as given in [3] and [4]. However in this case it is more elementary to work from the ideas in [5], and especially the appendix to [5], due to David Brydges.

Now we require the reader to have some familiarity both with [5] and either [1] or Section 5 of [2]. Fortunately these are all rather short.

We consider an elegant generalization of the setup in [5]. We replace the configuration space of a single particle, $\mathbb{R}^3$, with individual configurations, points $x \in \mathbb{R}^3$, by the space of two element subsets of $\mathbb{Z}^3$, with individual elements

$\{i,j\}$, subsets of $\mathbb{Z}^3$. The sum over one dimensional configurations, is changed from

$$\int dx$$

to

$$\sum_{\{i,j\}} v(i,j)$$

where v is as in (5.6) of [2] or (10) of [1]. Thus we are using the v's to weight the points of the new configuration space. Of the potentials in [5] we keep only V_r, given in the Appendix of [5], in eq (A1). It is constructed from v_{r2} a two-body potential as follows

$$v_{r2}\left(\{i,j\},\{k,l\}\right) = \left\{ \begin{array}{ll} 0 & \{i,j\} \cap \{k,l\} = \varnothing \\ +\infty & \text{otherwise} \end{array} \right. . \tag{45}$$

Then $u\left(\{i,j\},\{k,l\}\right)$ as defined in (A2) of [5] becomes

$$u\left(\{i,j\},\{k,l\}\right) = \left\{ \begin{array}{ll} 0 & \{i,j\} \cap \{k,l\} = \varnothing \\ -1 & \text{otherwise} \end{array} \right. . \tag{46}$$

A natural generalization of (6) of [5] is given by

$$\|u\| = \sum_{j \neq i} \left(\sum_{\{k,l\}} |v(k,l)| \, |u\left(\{i,j\},\{k,l\}\right)| \right) \tag{47}$$

where i is fixed.

It is easy to see from the definition of $v(i,j)$ that

$$\|u\| \leq 8 \tag{48}$$

since

$$\sum_j |v(i,j)| \leq 2. \tag{49}$$

The generalization of (56) of [5] becomes

$$|\bar{J}_n| \leq e^n 8^n. \tag{50}$$

(It is easy to improve this, replacing the right side of (50) by $2e^n 4^n$.)

For $d = 1$ the expansion in (5) holds for all $0 \leq p \leq 1$, as was noted at the end of [2]. We may expect this is true for all d!? The methods of the current paper do not get near this result. But the result we have encourages research to address this question. For that matter is $\lambda_d(p)$ analytic in both p and $1/d$ for $|1/d| < 1$, $|p| < 1$? Or on the other hand perhaps the result of this paper is essentially the best one can do!

References

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