the Dimer Gas Mayer Series, the Monomer-Dimer $\lambda_d(p)$, the Federbush Relation

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Abstract

The author and Shmuel Friedland recently presented an expression for $\lambda_d(p)$ of the monomer-dimer problem involving a power series in p . Herein I present a simple way to derive this expression for $\lambda_d(p)$ from the Mayer (or Virial) series of a dimer gas. The derivation is an exercise in basic statistical mechanics. We expect the relationship to be very useful.

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]. We always knew that the Mayer or Virial series of a dimer gas implicitly contained all the information to compute our series. (In [2], see the remark there in the paragraph following the paragraph containing eq. (30), the sentence beginning: "By a simple device...".) But it was not until the referee of a recent paper, [3], asked about the relationship of the expansion for $\lambda_d(p)$ to the Virial expansion that I finally worked out the details of the simple natural connection. We present the general development, and then specialize to $d = 2$ where the most is now known.

We take the statistical mechanical notation from Ruelle, [4]. We must be careful to avoid confusions, for example between the p in $\lambda_d(p)$ and pressure. We at the outset specify some notation.

1) p (as in $\lambda_d(p)$) is considered the <u>density</u> of vertices covered by dimers.

2) ρ is the <u>density</u> of dimers. So

$$p = 2\rho. \tag{1}$$

3) P is <u>pressure</u>.

4) The <u>Mayer series</u> from [4], page 84 are

$$\beta P = \sum_{n=1}^{\infty} b_n z^n \tag{2}$$

and

$$\rho = \sum_{n=1}^{\infty} n b_n z^n. \tag{3}$$

We will set $\beta = 1$. But we choose to work with the density p so we replace (3) by

$$p = 2\sum_{1}^{\infty} n b_n z^n. \tag{4}$$

5) We solve (4) for $z = z(p)$ by iterating (from $z = 0$)

$$z = \frac{1}{2b_1} p - \sum_{2}^{\infty} \frac{n b_n}{b_1} z^n. \tag{5}$$

We then substitute $z = z(p)$ into the right side of (2), getting

$$P(p) = \sum_{1}^{\infty} b_n (z(p))^n \tag{6}$$

Written as a power series in p this is the Virial series.

Considering the partition function leading to the Mayer series, we note that in volume V the sum is dominated by terms with $\sim \rho V$ dimers, leading to the observation that

$$\lambda_d(p) = P(p) - \frac{p}{2}\ln(z(p)) \tag{7}$$

This is the Federbush relation. (But perhaps this equality already has some name?) We here assume that the expansion of the left side of this relation given in eq. (7.1) of [1] is consistent with this relation, 'as it certainly must be'. We leave the proof of this, 'which is just algebra', to another day. Later we will see that for $d = 2$ we have checked this to the p^7 power.

We look at $z(p)$ as derived above

$$z = \frac{p}{2b_1}(1 + F(p)) \tag{8}$$

where $F(p)$ is a power series in p without a constant term.We use (8) to get

$$\lambda_d(p) = P(p) - \frac{p}{2}\ln\left(\frac{p}{2b_1}\right) - \frac{p}{2}\ln(1 + F(p)) \tag{9}$$

$$= -\frac{p}{2}\ln(p) + \frac{p}{2}\ln(2d) + P(p) - \frac{p}{2}\ln(1 + F(p)) \tag{10}$$

We have used that $b_1 = d$. Aside from the first two terms with ln's, the last two terms in (10) are polynomial series in p.

For $d = 2$ we calculated as the principal part of our computer computations (in calculating the $\bar{J}_i$ defined in [1]) the values of the first 7 coefficients in the Mayer series of a dimer gas:

$$b_1 = 2 \tag{11}$$
$$b_2 = -7 \tag{12}$$
$$b_3 = \frac{116}{3} \tag{13}$$
$$b_4 = -\frac{521}{2} \tag{14}$$
$$b_5 = \frac{9812}{5} \tag{15}$$
$$b_6 = -\frac{47644}{3} \tag{16}$$
$$b_7 = \frac{945688}{7} \tag{17}$$

Equation (10) with the appropriate substitutions yields the same series as in [3], up to order p^7 in the power series. The computations are easy using Maple:

$$\begin{aligned}\lambda_2(p) \sim & \frac{1}{2}(p\ln(4) - p\ln p - 2(1-p)\ln(1-p) - p) + \frac{4}{2}\cdot\left(\frac{1}{2\cdot 1}\left(\frac{p}{4}\right)^2\right. \\ & \left. + \frac{1}{3\cdot 2}\left(\frac{p}{4}\right)^3 + \frac{7}{4\cdot 3}\left(\frac{p}{4}\right)^3 + \frac{41}{5\cdot 4}\left(\frac{p}{4}\right)^5 + \frac{181}{6\cdot 5}\left(\frac{p}{4}\right)^6 + \frac{757}{7\cdot 6}\left(\frac{p}{4}\right)^7\right)\end{aligned} \tag{18}$$

The current development should make it straightforward to prove that the expansion for $\lambda_d(p)$, which is given in (10), converges to the correct value for small enough p. We had previously proved in [5] that the series converged, but not necessarily to the correct value. But we do not see how to recover from the results of the current paper the detailed knowledge of the dependence on dimension d of the earlier derivation.

References

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

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