MONOMERS AND DIMERS

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We prove that the free energy of an arbitrary monomer-dimer system is analytic in the density and temperature for nonzero density, and hence that the system has no phase transition. This result can also be used to locate the $z=e^{2\beta h}$ roots of the Heisenberg ferromagnet or antiferromagnet at high temperature.

From time to time the monomer-dimer (MD) system is used as a model of a physical system,[1] but primarily it is interesting as the phototypical lattice statistical mechanics problem. Although the pure dimer (PD) problem can be solved for planar lattices,[2] nothing was heretofore known rigorously about the MD problem because no theorems and no exact solutions were available (except in one dimension where the problem is not very interesting).

In this note we present the outline of a complete theory of the subject which allows us to answer most questions of physical interest. Essentially, the only question left unanswered is the nature of the singularity, if any, as we approach the PD limit, the answer to which is surely lattice dependent and, therefore, complicated. Gaunt's series expansions[3] offer nonrigorous but convincing evidence of the existence and lattice dependence of this singularity. Otherwise, our theorems show that the free energy is analytic in the monomer density ρ and the temperature $T=(k\beta)^{-1}$. This had been conjectured before for specific lattices on the basis of numerical calculations.[3] We can also show that the correlation functions exist and enjoy the same analyticity properties. An appropriate variable in which to form a power series convergent for all $\rho>0$ is easily derived. In short, all that remains to be done in any specific problem is to use conventional graphical expansions to calculate coefficients on a computer. Admittedly, this procedure is likely to be impractical for small monomer densities unless one has a clear idea of the singularity at $\rho=0$.

We also show how the MD theory can be used to locate the $z=e^{2\beta h}$ roots of the Heisenberg and Ising ferromagnet and antiferromagnet at high temperature (h is the magnetic field).

To formulate the problem consider a lattice L consisting of N vertices and a set of $\binom{N}{2}$ non-negative bond weights w_{ij}. We can introduce T by setting $w_{ij}=\exp(-\beta J_{ij})$ for suitable real J_{ij}. L is said to be <u>articulated</u> if the vertices can be numbered so that $w_{12}, w_{23}, w_{34}, \cdots, w_{N-1,N}\neq 0$. L is said to be <u>bounded</u> by W if $\sum_j w_{ij}\leqslant W$ for all i. Dimers can be placed on pairs of vertices so that each vertex has at most one dimer. The weight of a covering by d dimers on (a,b), (c,d), $\cdots$ is $w_{ab}, w_{cd}, \cdots$, and Z_d is the sum of these weights for all possible d-dimer coverings. Uncovered vertices are regarded as being occupied by monomers having an activity x, so that the total MD partition function is

$$P_L(x)=\sum_{d=0}^{M} Z_d x^{N-2d}, \tag{1}$$

where M is the largest integer in $N/2$. Let $P_{L'}$ be the partition function for the lattice with vertex N (and its edges) removed and let $P_{L'}{}^k$ be the same when vertices N and k are removed. The key equation is

$$P_L(x)=xP_{L'}(x)+\sum_{k=1}^{N-1} w_{k,N} P_{L'}{}^k(x). \tag{2}$$

For $N=1$ or 2 the roots of $P_L(x)=0$ are imaginary. We are led to the following theorem whose proof involves a simple modification of the classical inductive argument (on N) appropriate to a Sturm sequence and which can easily be supplied by the reader. The proof of the bound on the roots does not appear to be standard but it requires merely an addition to the inductive hypothesis which, <u>in toto</u>, reads, "For all lattices of order N, (a) Theorem 1 is true; (b) for $x=i\alpha$ and $\alpha\geqslant 2W^{1/2}$, $P_{L'}(x)/P_L(x)=i\delta$ with $\delta\geqslant -W^{-1/2}$."

<u>Theorem 1.</u>

$$P_L(x)=\prod_{j=1}^{M}(x^2+b_j),\ N \text{ even}$$

$$=x\prod_{j=1}^{M}(x^2+b_j),\ N \text{ odd}, \tag{3}$$

where $0 \leqslant b_j < 4W$. The roots of $P_L = 0$ interlace those of $P_{L'} = 0$ and, if L is articulated, the roots strictly interlace and hence are simple.

The significance of this theorem is that $\ln P_L(x)$ is analytic in the right-hand plane and hence that no phase transition can occur. The simplicity of the roots will be needed later in connection with the Heisenberg and Ising models.

Corollary 1.

$$2\ln Z_d \geqslant \ln Z_{d-1} + \ln Z_{d+1} + \ln\frac{(M-d+1)(d+1)}{(M-d)d}. \quad (4)$$

This is merely a statement of Newton's inequality.[4] Its meaning is that even for a finite system the free energy per unit volume is a strictly convex function of the monomer (or dimer) density.

The grand free energy per unit volume is

$$-\beta F = N^{-1}\ln P_L(x), \quad (5)$$

and it is clearly analytic away from the cut, $(-2iW^{1/2}, 2iW^{1/2})$. To expand F near zero monomer density, the natural variable to use is $u = x^{-1}$. As F has singularities in the u plane along $(i/2W^{1/2}, i\infty)$ and $(-i/2W^{1/2}, -i\infty)$, a power series in u will have only a finite radius of convergence. To remedy this use $s = (2W^{1/2}u)^{-1}[-1 + (1+4Wu^2)^{1/2}]$ or $W^{1/2}u = s(1-s^2)^{-1}$ which maps the unit s disk conformally onto the u plane less the cuts. Thus one constructs the usual power series in u, rearranges in powers of s, and convergence for all real u is guaranteed.

The monomer density is defined as

$$\rho = xN^{-1}d\ln P_L(x)/dx. \quad (6)$$

It is easy to prove from (3) the following:

Theorem 2. The roots of $d\rho/dx = 0$ lie in

$$D = \{x: |x| < 2W^{1/2}, \pi/4 < \arg x < 3\pi/4 \text{ and } 5\pi/4 < \arg x < 7\pi/4\}.$$

The significance of this theorem is that the inverse function theorem guarantees a neighborhood of the positive ρ axis in which F, considered as a function of ρ, is analytic.

The dimers can also be thought of as hard-core particles on the line (or covering) graph of L. For example, if $w_{ij} = 1$ on the edges of a planar hexagonal lattice and zero otherwise, the MD problem is the same as the nearest-neighbor exclusion problem on a Kagome lattice. Our theorem tells us that there is no phase transition on the Kagome lattice as there is for the square lattice.[5] Using this point of view, however, we can modify the Ginibre-Penrose method[6] to yield a lower bound on the compressibility,

$$\beta\chi^{-1} \equiv -\beta\rho\partial F/\partial\rho = \rho^2[x d\rho(x)/dx]^{-1}. \quad (7)$$

By this method one first derives the inequality

$$dZ_d^{\,2} < Z_{d-1}\{(d+1)Z_{d+1} + 2WZ_d\}, \quad (8)$$

and then

$$\beta\chi^{-1} < \tfrac{1}{2}\rho^2[1 + 2Wx^{-2}]/(1-\rho). \quad (9)$$

(We wish to thank Professor J. Lebowitz for calling our attention to the fact that by treating the dimers as hard-core particles the theorems of Ref. 6 independently yield the same qualitative conclusion as Theorem 2, namely that F is real analytic in ρ.)

Other bounds which can be derived directly from (3) are

$$\tfrac{1}{2}\rho/(1-\rho) \leqslant \beta\chi^{-1} \leqslant \tfrac{1}{2}\rho^2 W/(1-\rho)^2\chi^2, \quad (10)$$

$$\rho(x) \geqslant [1 + Wx^{-2}]^{-1}. \quad (11)$$

Turning now to a generalization of Theorem 1, we may consider a system in which placing a monomer at vertex i entails a Boltzmann factor $m_i x_i$ (instead of merely x) where $m_i > 0$, all i, and are regarded as fixed and x_i is the (variable) activity at site i. In this case we say that L is bounded by W if $m_i^{-1}\sum_j W_{ij} m_j^{-1} \leqslant W$ for all i.

Theorem 3. If $x_i = x$ for all i then Theorem 1 is still true. Otherwise, if $\mathrm{Re}(x_i) > 0$, all i, or $\mathrm{Re}(x_i) < 0$, all i, then $P_L(x_i, \cdots, x_N) \neq 0$. The proof is an adaptation of that for Theorem 1.

If w_{ij} depends on temperature, as aforementioned, analyticity in x does not trivially imply analyticity in β. The problem is similar to that for the Ising ferromagnet where the circle theorem holds.[7] Following the sophisticated analytic tour de force of Lebowitz and Penrose,[8] however, we can likewise show that for the MD problem there is analyticity in (x, β) for x in the right-hand plane and β real and positive. As they did, we can also establish the existence of correlation functions. These statements are, of course, trivial for a finite system. The difficulty lies in proving them in the thermodynamic $(N\to\infty)$ limit. To our knowledge, no one has ever carried out the proof of the convergence of the virial series for the MD problem, but this can be done in a manner parallel to that for the Ising model. Hammersley has, however, proved the existence of the thermodynamic limit.[9]

The analogy with the Ising circle theorem is not fortuitous. Fisher[10] has shown how a zero-field Ising model can be put into one-one correspondence with a PD problem, and with non-negative bond weights in the case of a ferromagnet. He did not show how to include a magnetic field, but that lack is easily filled with the result that the Ising model becomes a MD problem with $x = (z-1)/(z+1)$, $z = e^{2\beta h}$. The only difference is that not all sites are allowed to have monomers (i.e., $m_i = 0$ or 1 in the above) so that Theorem 3 is called into play. In brief, our analysis starting with (3) and using the notion of a Sturm sequence provides a completely independent proof of the circle theorem (note that $|z| = 1$ is equivalent to x imaginary).

On the other hand, we can start with the circle theorem and derive Theorem 1, except for the statement about the simplicity of the roots. For generality, consider a spin-$\frac{1}{2}$ Heisenberg Hamiltonian: $H = H_0 + H_1$; $H_0 = \sum J_{ij} s_{iz} s_{jz}$; H_1 = arbitrary Hermitian quadratic form in $\{s_{ix}, s_{iy}\}$, and let

$$Z = (e^{\beta h} + e^{-\beta h})^{-N} \operatorname{Tr}[\exp(-\beta H) \exp(2\beta h \sum s_{iz})].$$

Next, expand $e^{-\beta H}$ in a Taylor series, take the trace term by term, and express the result as an even polynomial of order N in $y = (e^{2\beta h} - 1)/(e^{2\beta h} + 1)$. If $c_{2k}(\beta)$ be the coefficient of y^{2k} in Z then $c_{2k}(\beta) = \beta^k Z_k + r_{2k}(\beta)$ where Z_k is the k-dimer partition function on a lattice in which $w_{ij} = J_{ij}$. The significant fact, which the reader can easily verify, is that r_{2k}, while complicated, is of higher order in β than k. Hence,

$$Z = t^{-N} P_L(t) + R_L(t), \tag{12}$$

where $t^{-2} \equiv \beta y^2$ and $R_L(t)$ is a polynomial whose coefficients all vanish with β. If $H_1 = 0$ (Ising model) and $J_{ij} \geq 0$, the circle theorem tells us that the roots of Z (in t) are imaginary for all positive β. It is easy to prove that the leading polynomial, $P_L(t)$, must necessarily also have this property and thus we have another proof of most of Theorem 1. Conversely, if the roots of $P_L(t)$ are imaginary and simple, Z will also have this property for sufficiently small β. If we also note that negating the sign of all J_{ij} is the same as changing t to it in P_L we have the following:

Theorem 4. Let H be the Hamiltonian of a Heisenberg ferromagnet ($J_{ij} \geq 0$) or antiferromagnet ($J_{ij} \leq 0$) such that the lattice of $\{J_{ij}\}$ is articulated. Then there exists a $\beta_0 > 0$ such that for $\beta < \beta_0$ the roots of $Z = 0$ in $e^{2\beta h}$ are (i) on the unit circle for a ferromagnet and (ii) on the negative real axis for an antiferromagnet.

Theorem 4 complements Suzuki's proof[11] of the circle theorem for sufficiently large β but, unlike his hypothesis, we are not obliged to place any constraint on the off-diagonal part, H_1. As in Suzuki's case, we are obliged to state that we can give no bound for β_0 which is independent of N.

After this work was completed, we received a preprint from T. Asano[12] which contains a complete proof of the circle theorem for the anisotropic Heisenberg ferromagnet. Consequently, the ferromagnetic part of our Theorem 4 is obsolete.

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[1]See, e.g., R. H. Fowler and G. S. Rushbrooke, Trans. Faraday Soc. 33, 1272 (1937).

[2]P. W. Kasteleyn, in *Graph Theory and Theoretical Physics*, edited by F. Harary (Academic, New York, 1967), p. 43. In certain cases the correlation functions for a few monomers in otherwise infinite sea of dimers can also be calculated: M. E. Fisher and J. Stephenson, Phys. Rev. 132, 1411 (1963); R. E. Hartwig, J. Math. Phys. 7, 286 (1966).

[3]D. S. Gaunt, Phys. Rev. 179, 174 (1969); L. K. Runnels, J. Math. Phys. 11, 849 (1970); J. F. Nagle, Phys. Rev. 152, 190 (1966); R. J. Baxter, J. Math. Phys. 9, 650 (1968).

[4]G. H. Hardy, J. E. Littlewood, and G. Polya, *Inequalities* (Cambridge Univ., Cambridge, England, 1959), Theorem 144.

[5]R. L. Dobrushin, Funktsional Analiz i Ego Prilozhen 2, 44 (1968) [Funct. Anal. Appl. 2, 302 (1968)].

[6]Cf. D. Ruelle, *Statistical Mechanics* (Benjamin, New York, 1969), Proposition (3.4.9).

[7]T. D. Lee and C. N. Yang, Phys. Rev. 87, 410 (1952).

[8]J. L. Lebowitz and O. Penrose, Commun. Math. Phys. 11, 99 (1968).

[9]J. M. Hammersley, in *Research Papers in Statistics; Festschrift in Honor of Jerzy Neyman*, edited by Florence Nightingale David and Evelyn Fix (Wiley, New York, 1966), p. 125.

[10]M. E. Fisher, J. Math. Phys. 7, 1776 (1966).

[11]M. Suzuki, Progr. Theoret. Phys. (Kyoto) 41, 1438 (1969).

[12]T. Asano, "The Rigorous Theorems for the Heisenberg Ferromagnet," (to be published).