A Combinatorial Solution of the Two-Dimensional Ising Model

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An elementary method which yields the partition function of a two-dimensional Ising model is described. The method is purely combinatorial and does not involve any of the algebraic apparatus used in this connection by Onsager and Kaufman.

I. INTRODUCTION

THE partition function of the two-dimensional square net Ising model can be easily put in the form[1]

$$(\cosh H)^h(\cosh H')^v\sum g(l,k)x^l y^k, \tag{1.1}$$

where

$$H=J/kT,\quad H'=J'/kT,\quad x=\tanh H,\quad g=\tanh H',$$

h the total number of horizontal links, v the total number of vertical links, and $g(l,k)$ the number of "closed polygons" with l horizontal and k vertical links. The problem is thus purely combinatorial and consists in counting closed polygons. Since the exact evaluation of the partition function was provided by Onsager[2] and Kaufman,[3] it seemed desirable to understand how the algebraic method of these authors performs the actual counting. This was the starting point of the present investigation. The authors felt that the exact formulas (for finite lattices) of Onsager and Kaufman should provide a clue to the proper method of counting and thus lead to an elementary combinatorial approach to the problem.

In the main body of the paper we shall explain in detail the method of counting which yields the partition function up to negligible terms due to boundary effects. Several combinatorial points will be dealt with a heuristic manner only. We do not go into the details of rigor because our main aim is not so much an alternative derivation of the Onsager-Kaufman formula but a demonstration that a combinatorial approach is indeed possible. Furthermore, the combinatorial approach provides a new insight into the problem and its difficulties. Although this new insight makes the three-dimensional Ising model look even more formidable than before, the authors hope that the method may find other useful application.

II. PRELIMINARIES

The exact formula for the partition function of an $n\times m$ lattice (wound on a torus) was found by Kaufman (see reference 3) to be of the form

$$Z=\frac{1}{2}\frac{(\sinh 2H)^{\frac{1}{2}mn}}{2^{\frac{1}{2}mn}}\left\{\prod_{r=1}^{n}\left(2\cosh\frac{m}{2}\gamma_{2r}\right)+\prod_{r=1}^{n}\left(2\sinh\frac{m}{2}\gamma_{2r}\right)+\prod_{r=1}^{n}\left(2\cosh\frac{m}{2}\gamma_{2r-1}\right)+\prod_{r=1}^{n}\left(2\sinh\frac{m}{2}\gamma_{2r-1}\right)\right\}, \tag{2.1}$$

where

$$\cosh\gamma_j=\cosh 2H^*\cosh 2H'-\sinh 2H^*\sinh 2H'\cos(\pi j/n),$$

or, equivalently,

$$\cosh\gamma_j=\frac{(1+x^2)(1+y^2)}{2x(1-y^2)}-\frac{(1-x^2)}{2x}\frac{2y}{1-y^2}\cos\frac{\pi j}{n}. \tag{2.2}$$

It is apparent that the complexity of formula (2.1) is due to taking boundary effects too seriously. For large lattices one expects the asymptotic formula

$$Z\sim\left(\frac{\sinh 2H}{2}\right)^{\frac{1}{2}mn}\prod_{r=1}^{n}\left(2\cosh\frac{m}{2}\gamma_{2r}\right),$$

which with the aid of the obvious relation,

$$\cosh l\theta=2^{l-1}\prod_{S=0}^{l-1}\left(\cosh\theta-\cos\frac{(2S+1)\pi}{2l}\right),$$

can be written as

$$Z\sim(\sinh 2H)^{ln}\prod_{r=1}^{n}\prod_{S=0}^{l-1}\left(\cosh\gamma_{2r}-\cos\frac{(2S+1)\pi}{2l}\right).$$

Here we set $m/2=l$ and assume that m is even. Making use of (2.2) one gets, after a few simple transformations,

$$Z\sim(\cosh H)^h(\cosh H')^v\prod_{r=1}^{n}\prod_{S=0}^{l-1}\left\{(1+x^2)(1+y^2)-2y(1-x^2)\cos\frac{2\pi r}{n}-2x(1-y^2)\cos\frac{(2S+1)\pi}{2l}\right\}.$$

For large lattices one can replace $(2S+1)$ by $2S$ and obtain finally

$$Z\sim(\cosh H)^h(\cosh H')^v\prod_{r=1}^{n}\prod_{S=1}^{\frac{1}{2}m}\left\{(1+x^2)(1+y^2)-2y(1-x^2)\cos\frac{2\pi r}{n}-2x(1-y^2)\frac{2\pi S}{m}\right\}. \tag{2.3}$$

[1] B. L. van der Waerden, Z. Physik **118**, 473 (1941).
[2] L. Onsager, Phys. Rev. **65**, 117 (1944).
[3] B. Kaufman, Phys. Rev. **76**, 1232 (1949).

(It may be pointed out that for a $n\times m$ lattice wound on a torus one has $h=v=mn$.) If one compares (2.3) with (1.1) one sees that, apart from boundary effects, one must have

$$\sum g(l,k)x^l y^k = \prod_{r=1}^{n}\prod_{S=1}^{\frac{1}{2}m}\left\{(1+x^2)(1+y^2) - 2y(1-x^2)\cos\frac{2\pi r}{n} - 2x(1-y^2)\cos\frac{2\pi S}{m}\right\}. \quad (2.4)$$

III. THE PRINCIPLE OF THE METHOD

The way we propose to attack the problem is to construct a suitable determinant[4] with ones (1's) on the main diagonal and x's, y's, and 0's off the main diagonal. The construction would have to be such that to each nonvanishing term in the expansion of the determinant there would correspond a unique closed polygon and vice versa. If the signs of the terms in the expansion of the determinant could all be made positive, the value of the determinant would yield the generating function $\sum g(l,k)x^l y^k$. This approach meets immediately with several difficulties which we find instructive to discuss before writing down the actual determinant. A determinant with ones on the main diagonal,

$$\begin{vmatrix} 1 & A_{12} & A_{13} & \cdots & \cdots & A_{1p} \\ A_{21} & 1 & A_{23} & \cdots & \cdots & A_{2p} \\ A_{31} & A_{32} & 1 & A_{34} & \cdots & A_{3p} \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ A_{p1} & A_{p2} & \cdot & \cdot & \cdot & 1 \end{vmatrix},$$

can be expanded as follows:

$$\sum \pm (A_{i_1 i_2} A_{i_2 i_3}\cdots A_{i_{s(1)} i_1})(A_{j_1 j_2}\cdots A_{j_{s(2)} j_1}) \cdots (A_{l_1 l_2}\cdots A_{l_{s(r)} l_1}). \quad (3.1)$$

The permutations of indices involved in these terms are products of cycles, and herein lies our hope of dentifying the terms of the expansion with closed polygons. In brief, we expect to identify closed polygons

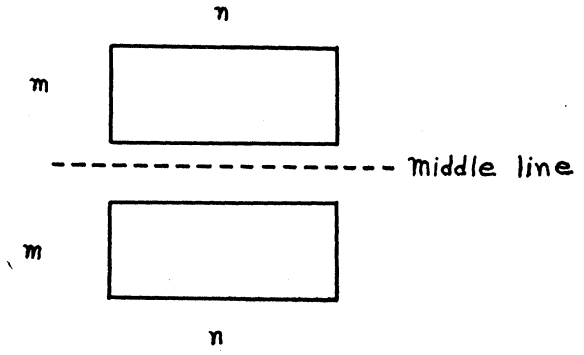

FIG. 1.

[4] We understand that Mr. Madox of Manchester University, England, has considered a similar idea. However, we are not aware of any publications on this subject.

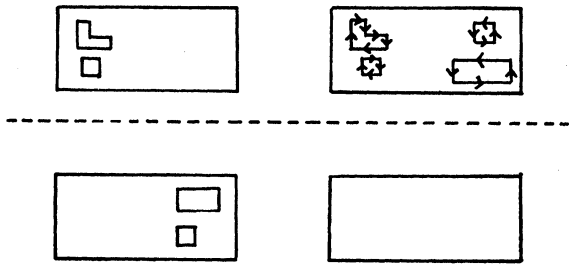

FIG. 2.

with cycles or, in case of closed polygons of several components, with products of cycles. We can now state the first difficulty which our approach encounters. If there is to be a one-to-one correspondence between terms in the expansion (3.1) and closed polygons, then terms like $A_{12}A_{23}A_{34}A_{41}$ and $A_{21}A_{14}A_{43}A_{32}$ should correspond to different closed polygons. On the other hand, the cycles involved in both of these terms, namely, (1234) and (2143), are inverses of each other and should be associated with the same polygon. It would thus seem that the determinant will, at best, count oriented polygons, whereas we are interested in the unoriented ones. This difficulty can be resolved by the following trick. Consider an $n\times 2m$ lattice (Fig. 1) and classify all closed polygons (unoriented) on this lattice into those which do and those which do not cut the middle line (dividing the $n\times 2m$ lattice into $2n\times m$ lattices). Disregarding the closed polygons which cut the middle line, we can associate with every other polygon an oriented polygon on the upper lattice by the following rule: The parts of the polygon in the upper lattice (if any) remain there and are oriented clockwise whereas the parts of the polygon in the lower lattice (if any) are replaced by their reflections through the middle line and are oriented counter-clockwise (Fig. 2). On the basis of this rule we can see that the generating function of unoriented closed polygons on the $n\times 2m$ lattice is equal (up to boundary effects due to neglecting figures which cut the middle line) to the generating function of oriented polygons on the $n\times m$ lattice.

Since the partition function for an $n\times 2m$ lattice is (in the limit as n and m become simultaneously infinite) the square of the partition function for an $n\times m$ lattice, we should expect the product,

$$\prod_{r=1}^{n}\prod_{S=1}^{m}\left\{(1+x^2)(1+y^2) - 2y(1-x^2)\cos\frac{2\pi r}{n} - 2x(1-y^2)\cos\frac{2\pi S}{m}\right\}, \quad (3.2)$$

to be the generating function of oriented closed polygons on the $n\times m$ lattice. There is, however, one more difficulty. The oriented polygon [Fig. 3(a)] does not correspond to any unoriented polygon, whereas the

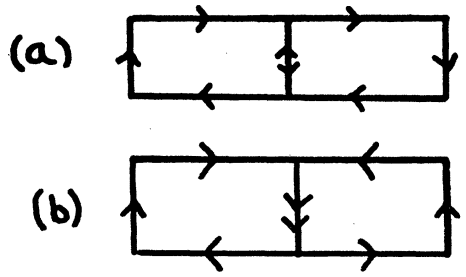

FIG. 3.

oriented polygon [Fig. 3(b)] does. This difficulty seems to spoil the one-to-one correspondence established above, but it can be resolved in the actual construction of the determinant. It will turn out that there will be no terms in the expansion of the determinant corresponding to figures like (b), whereas figures like (a) will be counted in a regular fashion. The fact that it is the "impossible" ones that one counted rather than the "possible" ones is of no consequence since, for counting purposes, the distinction is immaterial.

It should be noted finally that n and m enter symmetrically in (3.2), whereas in the Kaufman-Onsager formula they do not. This fact makes it apparent that the oriented closed polygons are the natural ones with which to deal. This in turn lends support to the naturalness of the determinant method because it is in this way that one is forced into considering oriented polygons.

IV. CONSTRUCTION OF THE DETERMINANT. FURTHER DIFFICULTIES AND THEIR RESOLUTION

We shall illustrate the construction of the determinant by considering a 4×4 lattice. The generalization to arbitrary size is easy and will be left to the reader. The oriented polygon shown in Fig. 4 is described as follows: (1.2)RD(2,6)DD(6,10)DL(10,9)LU(9,5)UU(5,1)UR(7,11)DR(11,12)RU(12,8)UL(8,7)LD. The numbers indicate which neighboring points are connected; the first of the letters R, L, D, U (Right, Left, Down, Up) indicates the direction in which the line joining the points is traversed, and the second letter the subsequent direction of motion. Symbols like (1,3) RD will not enter in describing closed polygons because 1 and 3 are not nearest neighbors. Neither will symbols like (1,2) RL and many others. Symbols like these will be called *improper*.

Let us now define a matrix $A_{(i,j)XY}$ $(i,j=1,2,3,4;$ $XY=$R, L, U, D) as follows:

$$\begin{aligned}&A_{(i,j)XY}=0 \text{ if } (i,j)XY \text{ is improper;}\\ &A_{(i,j)XY}=x \text{ if } X=\text{R or L (and the symbol is proper);}\\ &A_{(i,j)XY}=y \text{ if } X=\text{U or D (and the symbol is proper).}\end{aligned} \tag{4.1}$$

On the main diagonal we put ones (1's). The rows and columns are labeled as follows:

R	L	R	L	D
1 2 3 4	1 2 3 4	13 14 15 16	13 14 15 16	1 5 9 13

U	D	U
1 5 9 13	4 8 12 16	4 8 12 16

With x's and y's placed according to (4.1) we see that to each oriented closed polygon there corresponds a term

$$\pm x^l y^k \tag{4.2}$$

in the expansion of the determinant, where l and k denote, respectively, the number of horizontal and vertical lines in the polygon. We must first modify the matrix elements in such a way as to get only positive signs in (4.2). We note that the sign of a cycle of length C is $(-1)^{C-1}$, and since we are dealing with cycles of even length the sign is always negative. If a polygon consists of r components, so that the corresponding permutation is a product of r cycles, the sign will be $(-1)^r$. The modification of matrix elements must be accomplished in such a way as to provide a minus sign for each one-component polygon. This is done by multiplying each x and y by

$$\alpha=e^{\frac{1}{4}i\pi},\quad \alpha^{-1}=e^{-\frac{1}{4}i\pi},\quad \text{or}\quad \alpha^0=1,$$

according as the turning which is described by letter indices is through $\frac{1}{2}\pi$ (counter-clockwise), $-\frac{1}{2}\pi$ (clockwise), or 0. Thus, terms with indices RR, LL, UU, DD will remain unaltered, those with indices RU, UL, LD, DR will be multiplied by α, and those with indices RD, DL, LU, UR by α^{-1}. If we now take a closed one-component polygon, the term in the expansion of the modified determinant will be

$$(-1)^{\Omega/2\pi}(-1)x^l y^k,$$

where Ω is the total angle through which one turns in

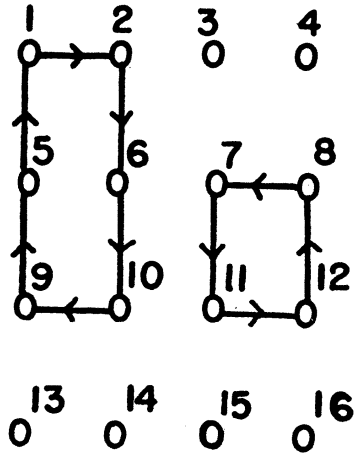

FIG. 4.

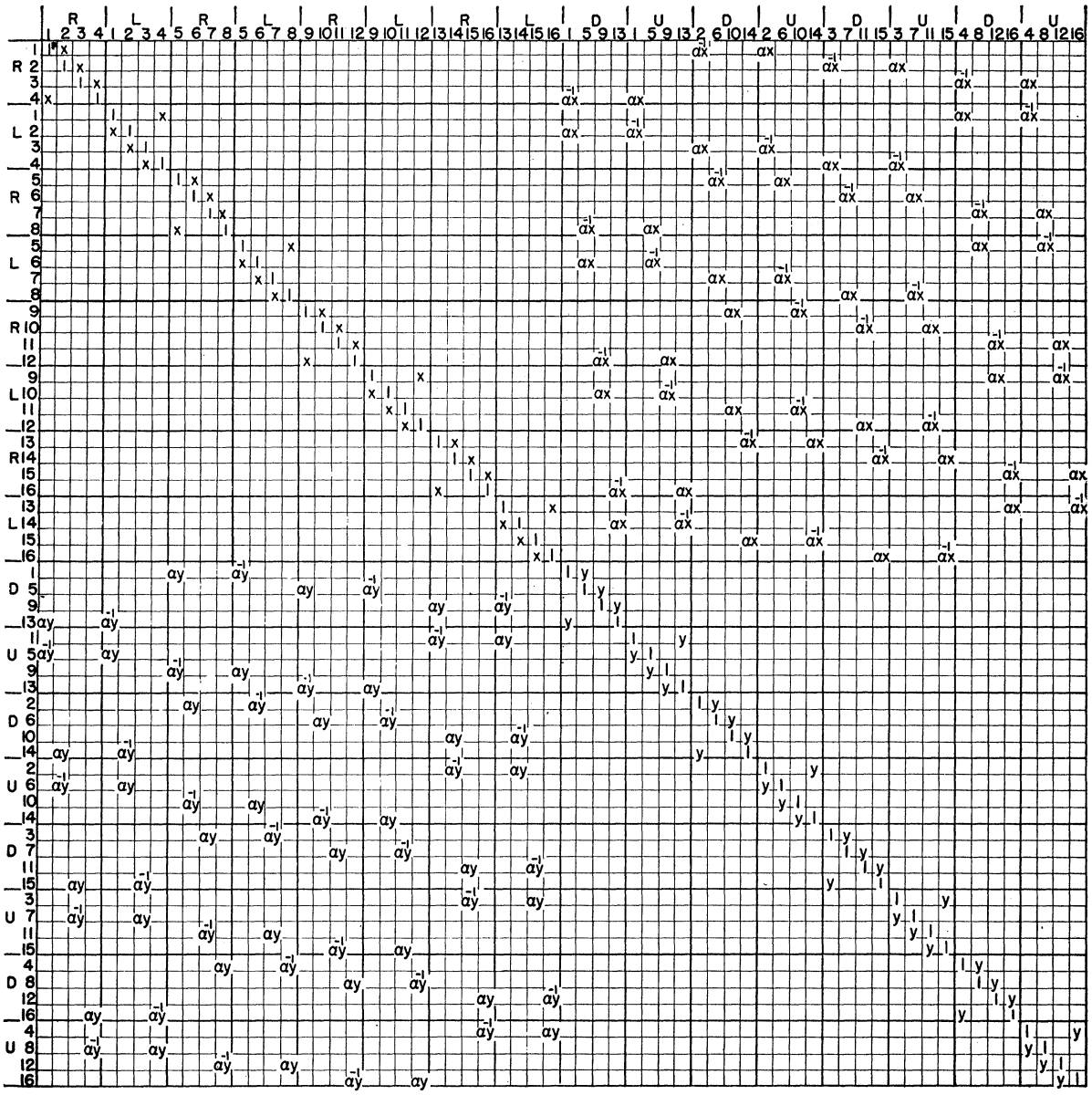

FIG. 5. The determinant for a 4×4 lattice.

describing the polygon. Since $\Omega=\pm 2\pi$, we get $+x^l y^k$ as desired.

The determinant is finally as given in Fig. 5.

Let us first see how the difficulty stated toward the end of Sec. 3 is resolved. Figure 6 is described symbolically as (1,2)RD(2,6)DL(6,5)LU(5,1)UR(2,3)LD(2,6)DR(6,7)RU(7,3)UL. This clearly does not correspond to any term in the expansion of our determinant because elements corresponding to (2,6)DL and (2,6)DR appear in the same row and only one element from each row is allowed.

There is finally one more difficulty, which fortunately resolves itself automatically. This difficulty is the following: There are terms in the expansion of our determinant which do not correspond to closed polygons. Some of these terms are trivial, like those which do not involve elements of the main diagonal or those like (1,2)RR(2,3)RR(3,4)RR(4,1)RR. The presence of these terms depends clearly on our decision to put the lattice on a torus, and hence they correspond to negligible boundary effects.

There are, however, also nontrivial terms. Such a nontrivial term can arise as shown in Fig. 6. Consider the closed polygon in Fig. 7, and note that it is a two-component figure and that hence it gives rise to 4 terms x^4y^4 corresponding to 4 distinct ways in which the two components can be traced out *separately*. But in the expansion of the determinant there will be 4

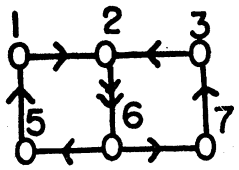

FIG. 6.

other terms which correspond to tracing out the polygon *unicursally*. We shall have terms corresponding to symbols:

(1,2)RD(2,6)DD(6,10)DR(10,11)RU(11,7)UL(7,6)LL (6,5)LU(5,1)UR,

(1,2)RD(2,6)DR(6,7)RD(7,11)DL(11,10)LU(10,6)UL (6,5)LU(5,1)UR,

and two more in which the directions of motion are reversed. The terms in the expansion of the determinant corresponding to these "unicursal" symbols cancel. To see this, note that in tracing out our polygon in the manner indicated by the first symbol we turn through the total angle 0, whereas in the second case the total angle is 2π. Since $(-1)^{0/2\pi}=1$ and $(-1)^{2\pi/2\pi}=-1$, the terms will be of opposite signs and will thus cancel each other. There is a general "topological" theorem which underlies this situation and which we state without proof:

Let there be $n(>1)$ plane closed curves such that each curve has a point in common with at least one other curve (Fig. 8). Then $\sum e^{i\Omega/2\pi}=0$, where the summation is extended over all unicursal ways of tracing out the resulting figure and Ω denotes the total angle through which one turns in a particular tracing.

The reader is invited to check other situations, like that in Fig. 9, and see how the cancellation follows from the above theorem. We thus arrive at the conclusion that our determinant is equal, except for boundary effects, to the generating function of the number of closed polygons. It should be clear that the considerations of this section apply to lattices of arbitrary size. We have chosen the 4×4 case just as a convenient illustration. For an $n\times m$ lattice the determinant is $4mn\times4mn$.

V. THE EVALUATION OF THE DETERMINANT

An examination of the determinant reveals that it has a certain amount of cyclic structure, and consequently it is not too difficult to guess the eigenvectors of the corresponding matrix.[5] Let ϵ and δ be two 4th roots of unity and consider the vector whose components are as follows: The first 32 components are obtained by multiplying the numbers $1, \epsilon, \epsilon^2, \epsilon^3$ by $a, b, a\delta, b\delta, a\delta^2, b\delta^2, a\delta^3, b\delta^3$, and repeating them in consecutive groups of four. The remaining 32 components are similarly obtained by multiplying the numbers $1, \delta, \delta^2, \delta^3$ by $c, d, c\epsilon, d\epsilon, c\epsilon^2, d\epsilon^2, c\epsilon^3, d\epsilon^3$. The components are thus $a, a\epsilon, a\epsilon^2, a\epsilon^3, b\delta, b\delta\epsilon, b\delta\epsilon^2, b\delta\epsilon^3, \cdots, d\epsilon^3, d\epsilon^3\delta, d\epsilon^3\delta^2, d\epsilon^3\delta^3$. In order that this vector be an eigenvector of our

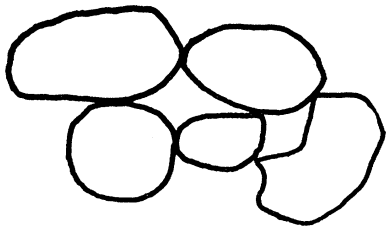

FIG. 8.

matrix it is easily seen that the following four linear equations must be satisfied:

$$\begin{aligned}(1+x\epsilon)a+0b+\alpha^{-1}x\epsilon c+dx\epsilon d&=\lambda a,\\ 0a+(1+x\epsilon^{-1})b+\alpha x\epsilon^{-1}c+\alpha^{-1}x\epsilon^{-1}d&=\lambda b,\\ dy\delta a+\alpha^{-1}y\delta b+(1+y\delta)c+0d&=\lambda c,\\ \alpha^{-1}y\delta^{-1}a+\alpha y\delta^{-1}b+0c+(1+y\delta^{-1})&=\lambda d.\end{aligned}\tag{5.1}$$

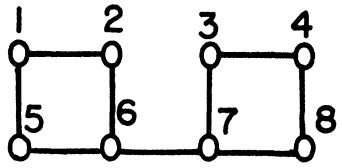

FIG. 9.

From these equations we get four eigenvalues $\lambda_1(\epsilon,\delta)$, $\lambda_2(\epsilon,\delta)$, $\lambda_3(\epsilon,\delta)$, $\lambda_4(\epsilon,\delta)$, and it is seen immediately that

$$\prod_{j=1}^{4}\lambda_j(\epsilon,\delta)=\begin{vmatrix}1+x\epsilon & 0 & \alpha^{-1}x\epsilon & \alpha x\epsilon\\ 0 & 1+x\epsilon^{-1} & \alpha x\epsilon^{-1} & \alpha^{-1}x\epsilon^{-1}\\ \alpha y\delta & \alpha^{-1}y\delta & 1+y\delta & 0\\ \alpha^{-1}y\delta^{-1} & \alpha y\delta^{-1} & 0 & 1+y\delta^{-1}\end{vmatrix}$$

$$=(1+x^2)(1+y^2)-y(1-x^2)(\epsilon+\epsilon^{-1})$$

$$-x(1-y^2)(\delta+\delta^{-1}).$$

The original determinant is the product of all eigen-

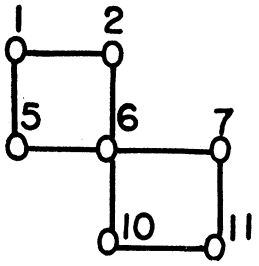

FIG. 7.

[5] After the determinant has been constructed and computed, several of our friends pointed out that a suitable reshuffling of rows and columns will reduce it to a form in which cyclicity is much more evident.

values and is thus equal to

$$\prod_{\epsilon,\delta}\prod_{j=1}^{4}\lambda_j(\epsilon,\delta)=\prod_{\epsilon,\delta}\{(1+x^2)(1+y^2)-y(1-x^2)(\epsilon+\epsilon^{-1})-x(1-y^2)(\delta+\delta^{-1})\},$$

which is precisely (2.4). Needless to say, in the $n\times n$ case ϵ and δ are nth roots of unity but the system of Eqs. (5.1) remains otherwise unchanged.

In conclusion, it is a pleasure to acknowledge the kind hospitality of The Institute for Advanced Study and to thank many of our friends for the healthy pessimism they showed during the early stages of this work.

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Magnetic Hyperfine Structure in Diatomic Molecules*,†

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A general theory of the magnetic hyperfine structure in diatomic molecules, including states other than $^1\Sigma$ states, is given. The magnetic hyperfine interaction is derived from the Dirac equation for the electron in the molecular potential field. First-order hyperfine structure formulas are given for the various vector coupling schemes characteristic of molecular states. The $^1\Sigma$ magnetic hyperfine structures are obtained from second order hyperfine interactions. Applications to the $N^{14}O^{16}$ and $O^{16}O^{17}$ microwave spectra are discussed.

1. INTRODUCTION

THE general theory of the nuclear hyperfine structure observed in atomic spectra has been worked out and discussed extensively,[1] and even the detailed features of the observed spectra are quite well understood. No such general treatment has apparently been given for diatomic molecules. In the case of diatomic molecules with no resultant electronic spin or orbital angular momentum ($^1\Sigma$), satisfactory phenomenological treatments of the magnetic interaction of the nuclear moment with the electronic currents, in the form of an $\mathbf{I}\cdot\mathbf{J}$ coupling with the molecular angular momentum vector, have been given.[2] Investigation has shown[3] that this effect arises for the most part from the effect in second order of the nondiagonal matrix elements of the nuclear magnetic interaction with the electronic currents. The interaction of the nuclear electric quadrupole moment with the electronic currents in these molecules has also been treated satisfactorily.[4] The development of microwave spectroscopy and molecular beam techniques have made it possible to examine the hyperfine spectra of paramagnetic gas molecules, i.e., molecules in states other than $^1\Sigma$. The present paper is devoted to the general treatment of the hyperfine spectra of diatomic molecules. For molecules with nonzero electronic angular momentum, it may be anticipated that the nuclear moment interaction with the electrons will be of the order of magnitude of atomic magnetic hyperfine couplings, and thus will be very much larger than typical nuclear electric quadrupole couplings. The strength and mode of the vector coupling of the nuclear spin to the various angular momentum vectors in the molecule will therefore be primarily determined by the magnetic interactions, and it will be sufficient in almost all cases to evaluate only the diagonal values of the electric quadrupole interaction, in a vector coupling representation determined by the magnetic interaction. The greater part of the present work will thus deal with the theory of the magnetic interaction of a single nuclear spin with the electronic currents in the various kinds of molecular states.

Typical features of the molecular magnetic hyperfine interactions may be compared with those of atoms. The interaction with electronic spins in the atomic case is treated quite differently in s states ($L=0$) and non-s states.[1] For non-s states, the spin coupling may be written as the interaction of two point magnetic dipoles in the form $3(\mathbf{I}\cdot\mathbf{R})(\mathbf{S}\cdot\mathbf{R})/R^5-(\mathbf{I}\cdot\mathbf{S})/R^3$, where $\mathbf{R}$ is the space vector from nucleus to electron. For s-states, this interaction vanishes (as does the orbital interaction), and the actual hyperfine coupling must be accounted for by a more refined treatment of the magnetic interaction. The most satisfactory method of treating the interaction of the nuclear magnetic moment with the electronic currents is via the Dirac equation for the

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† Assisted in part by the ONR.

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