Crystal Statistics of a Two-Dimensional Ising Lattice

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The partition function Z of a two-dimensional Ising lattice is evaluated by expressing it in the form $Z=\Sigma_i\lambda_i^{nm}$ where λ_i are the eigenvalues of a 2^n-dimensional matrix $\mathbf{M}$, n is the number of rows and m the number of columns of the lattice. $\mathbf{M}$ is a generalization of the V-shaped matrix studied by Kramers and Wannier in connection with the same problem. It is shown that $\mathbf{M}$ can be expressed in terms of 2^n-dimensional representations of $2n$-dimensional orthogonal matrices. The eigenvalues of $\mathbf{M}$ are determined for n large by making use of the known relations between the eigenvalues of a $2n$-dimensional orthogonal matrix and the eigenvalues of its 2^n-dimensional representative.

The lattice considered differs only slightly from that treated by Onsager and Kaufman. In the lattice considered here, the boundary effects are eliminated by introducing an interaction between the last lattice point of each row and the first point of the next row. The matrix $\mathbf{V}$ considered by Onsager and Kaufman is, except for the boundary effects, equivalent to the matrix $\mathbf{M}^n$. Z is shown to differ from the partition function calculated by Onsager and Kaufman only in order n^{-2}.

1. INTRODUCTION

THE partition function Z of a two-dimensional Ising lattice has been evaluated exactly by Onsager[1] and Kaufman.[2] The method used by them was to diagonalize a matrix $\mathbf{V}$ which represents the contribution to Z of a single *row* of lattice points. Kramers and Wannier[3] have shown that by a suitable choice of boundary conditions the partition function can also be expressed in terms of a matrix $\mathbf{M}$ which represents the contribution to Z of a single *point* of the lattice. This paper deals with the evaluation of Z according to the latter scheme. The two solutions will be shown to be equivalent in the limit of large crystals.

The model considered is a rigid two-dimensional rectangular lattice of m rows and n columns. To each lattice point is associated an "internal" coordinate μ_i which may assume the values $+1$ or -1 with equal *a priori* probabilities. The points of the lattice are numbered from 1 to $n\times m$ starting with the n points of the first row.[3] An interaction energy between a point and its nearest neighbor in a row is taken to be

$$-J\mu_j\mu_{j+1},$$

while that between a point and its nearest neighbor in a column is taken as

$$-J'\mu_j\mu_{j+n}.$$

The partition function for this model is:

$$Z=\sum_{\mu_i=\pm1}[\exp(J/kT\sum_{j=1}^{nm}\mu_j\mu_{j+1}+J'/kT\sum_{j=1}^{nm}\mu_j\mu_{j+1})]. \quad (1)$$

Included in this expression is a row type interaction $-J\mu_{in}\mu_{in+1}$ between the last point of one row and the first point of the next row; also a column interaction between the points of the mth row and those of the first row if

$$\mu_{nm+j}\equiv\mu_j.$$

[1] L. Onsager, Phys. Rev. **65**, 117 (1944).
[2] B. Kaufman, Phys. Rev. **76**, 1232 (1949).
[3] H. A. Kramers and G. H. Wannier, Phys. Rev. **60**, 252 (1941).

2. THE EIGENVALUE PROBLEM

A matrix $\mathbf{M}$ is defined by

$$M_{\mu_n'\mu_{n-1}'\cdots\mu_1',\,\mu_n\mu_{n-1}\cdots\mu_1}$$

$$\equiv\exp(H'\mu_n'\mu_n)\exp(H\mu_n'\mu_1)\prod_{j=1}^{n-1}\delta(\mu_j'-\mu_{j+1}), \quad (2)$$

where

$$H\equiv J/kT \quad H'\equiv J'/kT. \quad (3)$$

The index $\mu_n\mu_{n-1}\cdots\mu_1$ numbers the 2^n possible values of the coordinates $\mu_n, \mu_{n-1}, \cdots, \mu_1$.

Z is expressed in terms of this matrix as follows:

$$\left.\begin{aligned}Z=\sum_{\mu_i=\pm1}\prod_{i=1}^{nm}M_{\mu_{n+1}\cdots\mu_{i+1},\,\mu_{n+i-1}\cdots\mu_i}\\ =\text{trace }M^{nm}=\sum_{i=1}^{2^n}\lambda_i^{nm}\end{aligned}\right\}, \quad (4)$$

where λ_i are the 2^n eigenvalues of the matrix M.

The problem of evaluating Z is thus reduced to finding the eigenvalues of $\mathbf{M}$, the largest eigenvalues being particularly significant for large values of the product nm.

To simplify the notation, it is convenient to consider $\mathbf{M}$ as an operator operating on an orthogonal set of basis vectors $\psi(\mu_n\cdots\mu_1)$. To each state of the system with coordinates $\mu_n\cdots\mu_1$ is associated a state vector $\psi(\mu_n\cdots\mu_1)$. The operator $\mathbf{M}$ represented by the matrix (2) is defined by:

$$\mathbf{M}\psi(\mu_n,\cdots,\mu_1)$$

$$\equiv\sum_{\mu_i'=\pm1}M_{\mu_n'\cdots\mu_1',\,\mu_n\cdots\mu_1}\psi(\mu_n',\cdots,\mu_1'). \quad (5)$$

It will be shown that $\mathbf{M}$ can be written in the form

$$\mathbf{M}=\exp(H'\mathbf{s}_n\mathbf{s}_{n-1})(e^H+e^{-H}\mathbf{C}_n)\mathbf{R}, \quad (6)$$

where

$$\left.\begin{aligned}&\mathbf{R}\psi(\mu_n, \mu_{n-1}, \cdots, \mu_1)=\psi(\mu_1, \mu_n, \mu_{n-1}, \cdots, \mu_2)\\&\mathbf{C}_j\psi(\mu_n, \cdots, \mu_j, \cdots, \mu_1)=\psi(\mu_n, \cdots, -\mu_j, \cdots, \mu_1)\\&\mathbf{s}_j\psi(\mu_n, \cdots, \mu_j, \cdots, \mu_1)=\mu_j\psi(\mu_n, \cdots, \mu_j, \cdots, \mu_1)\end{aligned}\right\} \quad (7)$$

$$\mathbf{M}\psi(\mu_n\cdots\mu_1)=\exp(H'\mu_1\mu_n)e^{H}\psi(\mu_1, \mu_n, \cdots, \mu_2)$$
$$+\exp(-H'\mu_1\mu_n)e^{-H}\psi(-\mu_1, \mu_n, \cdots, \mu_2)$$

$$M_{\mu_n'\cdots\mu_1', \mu_n\cdots\mu_1}$$
$$=\exp(H'\mu_1\mu_n)e^{H}\delta(\mu_n'-\mu_1)\prod_{j=1}^{n-1}\delta(\mu_j'-\mu_{j+1})$$
$$+\exp(-H'\mu_1\mu_n)e^{-H}\delta(\mu_n'+\mu_1)\prod_{j=1}^{n-1}\delta(\mu_j'-\mu_{j+1})$$
$$=\exp(H'\mu_n\mu_n')\exp(H\mu_n'\mu_1)\prod_{j=1}^{n-1}\delta(\mu_j'-\mu_{j+1}),$$

which agrees with the definition (2).

Making the additional substitution of H^* defined by

$$e^{-2H}\equiv\tanh H^* \quad (8)$$

$\mathbf{M}$ takes the form

$$\mathbf{M}=(2\sinh 2H)^{\frac{1}{2}}\exp(H'\mathbf{s}_n\mathbf{s}_{n-1})\exp(H^*\mathbf{C}_n)\mathbf{R}. \quad (9)$$

The abstract properties of the operators (7) are as follows:

$$\left.\begin{aligned}&\mathbf{C}_j\mathbf{s}_k=\mathbf{s}_k\mathbf{C}_j \quad j\neq k && \mathbf{s}_j\mathbf{R}=\mathbf{R}\mathbf{s}_{j+1}\\&\mathbf{C}_j\mathbf{s}_j=-\mathbf{s}_j\mathbf{C}_j && \mathbf{C}_j\mathbf{R}=\mathbf{R}\mathbf{C}_{j+1}\\&\mathbf{C}_j\mathbf{C}_k=\mathbf{C}_k\mathbf{C}_j \quad \text{with} && \mathbf{s}_{n+j}\equiv\mathbf{s}_j\\&\mathbf{s}_j\mathbf{s}_k=\mathbf{s}_k\mathbf{s}_j && \mathbf{C}_{n+j}\equiv\mathbf{C}_j\\&\mathbf{C}_j^2=1, \ \mathbf{s}_j^2=1, \ \mathbf{R}^n=1\end{aligned}\right\}. \quad (10)$$

3. SPINOR REPRESENTATIVES OF THE ORTHOGONAL GROUP

Following a procedure similar to that used by Kaufman,[2] it will be shown that $\mathbf{M}$ can be written in terms of spinor representatives of the $2n$-dimensional orthogonal group. To do this we introduce a set of operators $\mathbf{\Gamma}_k$ satisfying the commutation rules

$$\mathbf{\Gamma}_k^2=1 \quad \mathbf{\Gamma}_k\mathbf{\Gamma}_l=-\mathbf{\Gamma}_l\mathbf{\Gamma}_k \quad 1\leq k, l\leq 2n. \quad (11)$$

A possible realization of these is given by[4]

$$\left.\begin{aligned}&\mathbf{\Gamma}_{2r-1}\equiv\mathbf{C}_1\mathbf{C}_2\cdots\mathbf{C}_{r-1}\mathbf{s}_r\equiv\mathbf{P}_r\\&\mathbf{\Gamma}_{2r}\equiv i\mathbf{C}_1\mathbf{C}_2\cdots\mathbf{C}_{r-1}\mathbf{C}_r\mathbf{s}_r\equiv\mathbf{Q}_r\end{aligned}\right\}. \quad (12)$$

In terms of these operators we have:

$$\left.\begin{aligned}&\mathbf{C}_r=i\mathbf{P}_r\mathbf{Q}_r \quad \mathbf{s}_1\mathbf{s}_n=i\mathbf{P}_1\mathbf{Q}_n\mathbf{U}\\&\mathbf{s}_{r+1}\mathbf{s}_r=-i\mathbf{P}_{r+1}\mathbf{Q}_r, \quad 1\leq r\leq n-1\\&\mathbf{U}\equiv\mathbf{C}_1\mathbf{C}_2\cdots\mathbf{C}_n\end{aligned}\right\}. \quad (13)$$

In order that some operator $\mathbf{S}(o)$ be a spin representative of a rotation in the $2n$-dimensional space whose basis vectors are the $2n$ $\mathbf{\Gamma}_k$'s, $\mathbf{S}(o)$ must satisfy the relation

$$\mathbf{S}(o)\mathbf{\Gamma}_k\mathbf{S}(o)^{-1}=\sum_{j=1}^{2n}o_{kj}\mathbf{\Gamma}_j\equiv\mathbf{\Gamma}_k^* \quad 1\leq k\leq 2n, \quad (14)$$

where o_{kj} is a (not necessarily real) orthogonal $2n$-dimensional matrix.

The correspondence between the orthogonal group o and the transformations $\mathbf{S}(o)$ is not one-to-one. If $\mathbf{S}(o)$ satisfies (14) so does $\rho\mathbf{S}(o)$ where ρ is any complex number. The arbitrariness of ρ can be partially removed by restricting $\mathbf{S}(o)$ to satisfy the additional conditions,[5]

$$\left.\begin{aligned}&\mathbf{N}^{-1}\mathbf{S}(o)\mathbf{N}=[\mathbf{S}^{-1}(o)]'\\&\mathbf{N}\equiv\mathbf{P}_1\mathbf{P}_2\cdots\mathbf{P}_n \quad \text{for } n \text{ even}\\&\quad\equiv\mathbf{Q}_1\mathbf{Q}_2\cdots\mathbf{Q}_n \quad \text{for } n \text{ odd}\end{aligned}\right\}. \quad (15)$$

where

A prime denotes the transposed matrix. The index ρ may still assume the values ± 1 giving a two-to-one correspondence $\pm\mathbf{S}(o)\leftrightarrow o$.

It can be shown[2] that if o has the $2n$-eigenvalues

$$e^{\pm i\theta_1}, e^{\pm i\theta_2}, \cdots, e^{\pm i\theta_n}; \quad (16)$$

then $\mathbf{S}(o)$ has the eigenvalues

$$(\pm)e^{i/2(\pm\theta_1\pm\theta_2\pm\cdots\pm\theta_n)}. \quad (17)$$

The 2^n-eigenvalues of $\mathbf{S}(o)$ are obtained by taking all possible combinations of plus and minus signs in the exponent and *one* of the two possible signs $(\pm)$ in front. One of the signs $(\pm)$ belongs to $\mathbf{S}(o)$, the other to $-\mathbf{S}(o)$. The knowledge that $\mathbf{S}$ is a representative of o having eigenvalues (16) is not in itself sufficient to determine the sign of (17).

The operators $\exp(H'\mathbf{s}_n\mathbf{s}_{n-1})=\exp(-iH'\mathbf{P}_n\mathbf{Q}_{n-1})$ and $\exp(H^*\mathbf{C}_n)=\exp(iH^*\mathbf{P}_n\mathbf{Q}_n)$ are examples of spin representatives since

$$\left.\begin{aligned}&\exp(\theta/2\mathbf{\Gamma}_k\mathbf{\Gamma}_l)\mathbf{\Gamma}_k\exp(-\theta/2\mathbf{\Gamma}_k\mathbf{\Gamma}_l)=\cos\theta\mathbf{\Gamma}_k-\sin\theta\mathbf{\Gamma}_l\\&\exp(\theta/2\mathbf{\Gamma}_k\mathbf{\Gamma}_l)\mathbf{\Gamma}_l\exp(-\theta/2\mathbf{\Gamma}_k\mathbf{\Gamma}_l)=\sin\theta\mathbf{\Gamma}_k+\cos\theta\mathbf{\Gamma}_l\\&\exp(\theta/2\mathbf{\Gamma}_k\mathbf{\Gamma}_l)\mathbf{\Gamma}_j\exp(-\theta/2\mathbf{\Gamma}_k\mathbf{\Gamma}_l)=\mathbf{\Gamma}_j \quad \mathbf{\Gamma}_j\neq\mathbf{\Gamma}_k\mathbf{\Gamma}_l,\end{aligned}\right\}. \quad (18)$$

$\mathbf{R}$ itself is not, however, such an operator. The $\mathbf{\Gamma}_k$ transform under $\mathbf{R}$ according to the following:

$$\left.\begin{aligned}&\mathbf{R}\mathbf{P}_r\mathbf{R}^{-1}=\mathbf{C}_n\mathbf{P}_{r-1}=i\mathbf{P}_n\mathbf{Q}_n\mathbf{P}_{r-1}\\&\mathbf{R}\mathbf{Q}_r\mathbf{R}^{-1}=\mathbf{C}_n\mathbf{Q}_{r-1}=i\mathbf{P}_n\mathbf{Q}_n\mathbf{Q}_{r-1}\end{aligned}\right\}2\leq r\leq n\Bigg\}, \quad (19)$$
$$\mathbf{R}\mathbf{P}_1\mathbf{R}^{-1}=\mathbf{C}_n\mathbf{U}\mathbf{P}_n, \quad \mathbf{R}\mathbf{Q}_1\mathbf{R}^{-1}=\mathbf{C}_n\mathbf{U}\mathbf{Q}_n$$

whereas the product of two $\mathbf{\Gamma}_k$'s transform according to

$$\left.\begin{aligned}&\mathbf{R}\mathbf{P}_r\mathbf{Q}_r\mathbf{R}^{-1}=\mathbf{P}_{r-1}\mathbf{Q}_{r-1} \quad 1\leq r\leq n\\&\mathbf{R}\mathbf{P}_{r+1}\mathbf{Q}_r\mathbf{R}^{-1}=\mathbf{P}_r\mathbf{Q}_{r-1} \quad 2\leq r\leq n-1\\&\mathbf{R}\mathbf{P}_1\mathbf{Q}_n\mathbf{R}^{-1}=-\mathbf{U}\mathbf{P}_n\mathbf{Q}_{n-1}, \quad \mathbf{R}\mathbf{P}_2\mathbf{Q}_1\mathbf{R}^{-1}=-\mathbf{U}\mathbf{P}_1\mathbf{Q}_n\end{aligned}\right\}. \quad (20)$$

The operators $\mathbf{\Gamma}_k$ belong to the group of operators which anticommute with $\mathbf{U}$ while $\mathbf{\Gamma}_j\mathbf{\Gamma}_k$ belong to the group of operators which commute with $\mathbf{U}$. $\mathbf{U}$ has the

[4] The product of two operators $\mathbf{AB}$ is used here to denote the result of operating first with $\mathbf{B}$ and then with $\mathbf{A}$. The product of the corresponding matrices is then $(AB)_{ac}=\sum_b A_{ab}B_{bc}$. This is apparently not the same convention as used by Kaufman.

[5] See R. Brauer and H. Weyl, Am. J. Math. **57**, 425 (1935); also F. D. Murnaghan, *The Theory of Group Representations* (The Johns Hopkins Press, Baltimore, 1938), Chapter 10.

eigenvalues $+1$ and -1 corresponding to the "even" and "odd" eigenfunctions

$$\left.\begin{aligned} &2^{-\frac{1}{2}}[\psi(\mu_n\cdots\mu_1)+\psi(-\mu_n,-\mu_{n-1},\cdots,-\mu_1)]\\ &\text{and}\\ &2^{-\frac{1}{2}}[\psi(\mu_n\cdots\mu_1)-\psi(-\mu_n,-\mu_{n-1},\cdots,-\mu_1)]\end{aligned}\right\}, \quad (21)$$

respectively.

In the space of even and odd functions, $\mathbf{U}$ has the form

$$\mathbf{U}=\begin{pmatrix} I & 0\\ 0 & -I\end{pmatrix}, \quad (22)$$

where I stands for the 2^{n-1}-dimensional unit matrix. Since $\mathbf{P}_r\mathbf{Q}_r$, $\mathbf{P}_{r+1}\mathbf{Q}_r$ and $\mathbf{R}$ commute with $\mathbf{U}$, they must be of the form

$$\begin{pmatrix} x_+ & 0\\ 0 & x_-\end{pmatrix}. \quad (23)$$

The last two equations of (20) may be written

$$\mathbf{R}\mathbf{P}_1\mathbf{Q}_n\mathbf{R}^{-1}=\mp\mathbf{P}_n\mathbf{Q}_{n-1}, \quad \mathbf{R}\mathbf{P}_2\mathbf{Q}_1\mathbf{R}^{-1}=\mp\mathbf{P}_1\mathbf{Q}_n, \quad (20a)$$

where the upper sign applies in the space of even functions, and the lower sign in the space of odd functions.

Despite the fact that $\mathbf{R}$ is not a spin representative, we consider the spin representatives $\mathbf{A}_+$ and $\mathbf{A}_-$ defined by the relations

$$\left.\begin{aligned} &\mathbf{A}_\pm\mathbf{P}_r\mathbf{A}_\pm^{-1}=\mathbf{P}_{r-1}\\ &\mathbf{A}_\pm\mathbf{Q}_r\mathbf{A}_\pm^{-1}=\mathbf{Q}_{r-1}\end{aligned}\right\}2\le r\le n \qquad \left.\begin{aligned} &\mathbf{A}_\pm\mathbf{P}_1\mathbf{A}_\pm^{-1}=\mp\mathbf{P}_n, \quad \mathbf{A}_\pm\mathbf{Q}_1\mathbf{A}_\pm^{-1}=\mp\mathbf{Q}_n\end{aligned}\right\}. \quad (24)$$

$\mathbf{A}_+$ and $\mathbf{A}_-$ also commute the $\mathbf{U}$ and so can be represented in the block form (23).

We note that $\mathbf{A}_+^{-1}\mathbf{R}$ commutes with all elements of the form $\mathbf{P}_r\mathbf{Q}_r$, $\mathbf{P}_{r+1}\mathbf{Q}_r$ (or equivalently $\mathbf{C}_r$, $\mathbf{s}_r\mathbf{s}_{r+1}$) in the 2^{n-1}-dimensional space of even functions while $\mathbf{A}_-^{-1}\mathbf{R}$ commutes with these elements in the space of odd functions.

The operators $\mathbf{C}_r$, $\mathbf{s}_{r+1}\mathbf{s}_r$ with $\mathbf{U}=1$ generate a group having but one faithful irreducible representation,[1] namely the 2^{n-1}-dimensional representation corresponding to the upper block of (23). Since $\mathbf{A}_+^{-1}\mathbf{R}$ commutes with every element of the group, it must be a multiple of the 2^{n-1}-dimensional unit matrix (in the space of even functions). By the same argument $\mathbf{A}_-^{-1}\mathbf{R}$ must be a multiple of the unit matrix in the space of odd functions. It follows that

$$\left.\begin{aligned} &[c_+^{-1}\tfrac{1}{2}(1+\mathbf{U})\mathbf{A}_+^{-1}+c_-^{-1}\tfrac{1}{2}(1-\mathbf{U})\mathbf{A}_-^{-1}]\mathbf{R}=I\\ &\mathbf{R}=c_+\tfrac{1}{2}(1+\mathbf{U})\mathbf{A}_++c_-\tfrac{1}{2}(1-\mathbf{U})\mathbf{A}_-\end{aligned}\right. \quad (25)$$

c_+ and c_- are constants. The operators $\frac{1}{2}(1+\mathbf{U})$ and $\frac{1}{2}(1-\mathbf{U})$ are projection operators into the space of even and odd functions, respectively.

c_+ and c_- can be determined only if $\mathbf{A}_\pm$ are uniquely defined. If $\mathbf{A}_+$ and $\mathbf{A}_-$ are restricted to satisfy condition (15) in addition to (24) then

$$\left.\begin{aligned} &c_+=\pm i, \quad c_-=\pm 1 \quad \text{for } n \text{ odd}\\ &c_+=\pm 1, \quad c_-=\pm i \quad \text{for } n \text{ even.}\end{aligned}\right.$$

$\mathbf{R}$ is uniquely defined by (7) whereas $\mathbf{A}_\pm$ is defined only to a sign by (24) and (15); therefore Eq. (25) can be used, in conjunction with (15) and (24), to define $\mathbf{A}_\pm$ uniquely by requiring that

$$\left.\begin{aligned} &c_+=-i, \quad c_-=1 \quad \text{for } n \text{ odd}\\ &c_+=1, \quad c_-=-i \quad \text{for } n \text{ even}\end{aligned}\right\}. \quad (26)$$

The operator $\mathbf{M}$ may now be written in the form

$$\left.\begin{aligned} &\mathbf{M}=(2\sinh 2H)^{\frac{1}{2}}[\tfrac{1}{2}(1+\mathbf{U})c_+\mathbf{M}_++\tfrac{1}{2}(1-\mathbf{U})c_-\mathbf{M}_-]\\ &\mathbf{M}_+\equiv\exp(-iH'\mathbf{P}_n\mathbf{Q}_{n-1})\exp(iH^*\mathbf{P}_n\mathbf{Q}_n)\mathbf{A}_+\\ &\mathbf{M}_-\equiv\exp(-iH'\mathbf{P}_n\mathbf{Q}_{n-1})\exp(iH^*\mathbf{P}_n\mathbf{Q}_n)\mathbf{A}_-\end{aligned}\right\}. \quad (27)$$

$\mathbf{M}_+$ and $\mathbf{M}_-$ are spin representatives of $2n$-dimensional orthogonal matrices. The eigenvalues of $\mathbf{M}$ can be found by selecting the eigenvalues of $\mathbf{M}_+$ belonging to the even space and the eigenvalues of $\mathbf{M}_-$ belonging to the odd space. The V-shaped matrix of Kramers and Wannier[3] corresponds to the first term of (27) with $H=H'$.

4. EIGENVALUES FOR M

According to the convention of multiplying operators and matrices (see reference 4), $\mathbf{S}(o)$ is to be associated with the matrix o' since

$$\mathbf{S}(o^*)\mathbf{S}(o)\boldsymbol{\Gamma}_k\mathbf{S}^{-1}(o)\mathbf{S}^{-1}(o^*)=\sum_{j,m=1}^{2n}o_{kj}o_{jm}{}^*\boldsymbol{\Gamma}_m=\sum_m(o^{*\prime}o')_{km}{}'\boldsymbol{\Gamma}_m. \quad (28)$$

The $2n$-dimensional transposed matrices $\mathfrak{M}_\pm$ to be associated with $\mathbf{M}_\pm$ are the products of the three transposed matrices

$$\begin{pmatrix} 1&0&0&\cdot&\cdot&\cdot&\cdot&&&\\ 0&1&0&\cdot&\cdot&\cdot&\cdot&&&\\ 0&0&1&\cdot&\cdot&\cdot&\cdot&&&\\ \cdot&\cdot&\cdot&\cdot&\cdot&\cdot&\cdot&&&\\ &&&1&0&0&0&&&\\ &&&0&\cosh 2H'&i\sinh 2H'&0&&&\\ &&&0&-i\sinh 2H'&\cosh 2H'&0&&&\\ &&&0&0&0&1&&&\end{pmatrix},$$

$$\begin{pmatrix} 1&0&0&\cdot&\cdot&\cdot&\cdot&&&\\ 0&1&0&\cdot&\cdot&\cdot&\cdot&&&\\ 0&0&1&\cdot&\cdot&\cdot&\cdot&&&\\ \cdot&\cdot&\cdot&\cdot&\cdot&\cdot&\cdot&&&\\ &&&&&&&1&0&0\\ &&&&&&&0&\cosh 2H^*&i\sinh 2H^*\\ &&&&&&&0&-i\sinh 2H^*&\cosh 2H^*\end{pmatrix}$$

and

$$\begin{pmatrix} 0&0&1&0&0&\cdot&\cdot&&&\\ 0&0&0&1&0&\cdot&\cdot&&&\\ 0&0&0&0&1&\cdot&\cdot&&&\\ \cdot&\cdot&\cdot&\cdot&\cdot&\cdot&\cdot&&&\\ 0&0&0&\cdot&\cdot&\cdot&\cdot&0&1&0\\ 0&0&0&\cdot&\cdot&\cdot&\cdot&0&0&1\\ \mp1&0&0&\cdot&\cdot&\cdot&\cdot&0&0&0\\ 0&\mp1&0&\cdot&\cdot&\cdot&\cdot&0&0&0\end{pmatrix}$$

corresponding, respectively, to the operators

$$\exp(-iH'\mathbf{P}_n\mathbf{Q}_{n-1}),\quad \exp(iH^*\mathbf{P}_n\mathbf{Q}_n)$$

and $\mathbf{A}_\pm$.

$$\mathfrak{M}_\pm=\begin{vmatrix} 0&0&1&0&0&\cdot&\cdot&\cdot&\cdot\\ 0&0&0&1&0&\cdot&\cdot&\cdot&\cdot\\ 0&0&0&0&1&\cdot&\cdot&\cdot&\cdot\\ \cdot&\cdot&\cdot&\cdot&\cdot&\cdot&\cdot&\cdot&\cdot\\ 0&0&0&\cdot&\cdot&\cdot&\cdot&1&0&0\\ 0&0&0&\cdot&\cdot&\cdot&\cdot&0&1&0\\ a&b&o&\cdot&\cdot&\cdot&\cdot&0&0&g\\ c&d&o&\cdot&\cdot&\cdot&\cdot&0&0&h\\ e&f&o&\cdot&\cdot&\cdot&\cdot&0&0&0 \end{vmatrix}, \tag{29}$$

where

$$\left.\begin{aligned} a&=\mp i\sinh 2H'\cosh 2H^* & e&=\pm i\sinh 2H^*\\ b&=\pm\sinh 2H'\sinh 2H^* & f&=\mp\cosh 2H^*\\ c&=\mp\cosh 2H'\cosh 2H^* & g&=\cosh 2H'\\ d&=\mp i\cosh 2H'\sinh 2H^* & h&=-i\sinh 2H' \end{aligned}\right\}. \tag{30}$$

Owing to the simplicity of the matrices $\mathfrak{M}_\pm$, the eigenvalues $m_\pm$ can be found for arbitrary n by solving the determinantal equation

$$D=\det(\mathfrak{M}_\pm-m_\pm I)=0.$$

I is the $2n$-dimensional identity. The result is

$$D=(m_\pm)^{2n}-b(m_\pm)^{n+1}-2c(m_\pm)^n-b(m_\pm)^{n-1}+1=0.$$

The substitution

$$m_\pm=e^z \tag{31}$$

gives the (complex) equation

$$\cosh nz=c+b\cosh z=\mp(\cosh 2H'\cosh 2H^*-\sinh 2H'\sinh 2H^*\cosh z). \tag{32}$$

For $z=x+iy$, this is equivalent to the two real equations

$$\cosh nx\cos ny=\mp(\cosh 2H'\cosh 2H^*-\sinh 2H'\sinh 2H^*\cosh x\cos y), \tag{32a}$$

$$\sinh nx\sin ny=\pm\sinh 2H'\sinh 2H^*\sinh x\sin y. \tag{32b}$$

For $n\gg 1$, it is possible to find z explicitly in the form of an expansion in powers of n^{-1}. In particular, if $n\to\infty$, the solution can be found as follows:

$$\sinh x/\sinh nx\to 0 \text{ thus } \sin ny\to 0$$
$$ny_j\to j\pi,\ j \text{ an integer} \tag{33}$$

(32a) then gives:

$$(-1)^j\cosh nx_j\to\mp(\cosh 2H'\cosh 2H^*-\sinh 2H'\sinh 2H^*\cos j\pi/n).$$

The factor $\cosh x$ has been replaced by 1 because this equation shows that nx_j is bounded as $n\to\infty$, therefore $x\to 0$. For a given choice of sign on the right, not all values of j are allowed. The function $\cosh nx$ is always positive as is the quantity in parentheses, therefore for the upper sign j must be odd, for the lower sign j must be even.

The $2n$-eigenvalues of $\mathfrak{M}_+$ and $\mathfrak{M}_-$ for $n\to\infty$ are:

$$\left.\begin{aligned} m_+&=\exp[\pm(x_{2r+1}+i(2r+1)\pi/n)];\quad m_-=\exp[\pm(x_{2r}+i2r\pi/n)]\\ &0\le r\le n-1,\quad r=\text{integer}\\ \cos nx_j&=\cosh 2H'\cosh 2H^*-\sinh 2H'\sinh 2H^*\cos j\pi/n \end{aligned}\right\}. \tag{34}$$

For arbitrary n, (32a,b) shows that if $z=x+iy$ is a solution then so are $\pm(x\pm iy)$. Also $y_0=0$ is a solution for $\mathfrak{M}_-$ and $y_n=\pi$ is a solution for $\mathfrak{M}_+$ if n is odd or for $\mathfrak{M}_-$ if n is even. In view of this we adopt the following convention for ordering the value of z:

$$\left.\begin{aligned} &\pm z_{2r+1}=\pm(x_{2r+1}+iy_{2r+1}) \text{ belong to } \mathfrak{M}_+\\ &\pm z_{2r}=\pm(x_{2r}+iy_{2r}) \text{ belong to } \mathfrak{M}_-\\ &x_j=x_{2n-j},\quad y_j=-y_{2n-1}\\ &-\pi<y_j\le\pi,\quad 0=y_0<y_1<y_2\cdots<y_n=\pi \end{aligned}\right\}\ 0\le r\le n-1\Bigg\}. \tag{35}$$

We also take x_j to be the positive solution of (32a,b) except in the case x_0 which will be considered in more detail later.

By (16) and (17), the eigenvalues of $\mathbf{M}_+$ are

$$(\pm)\exp[\tfrac{1}{2}(\pm z_1\pm z_3\pm z_5\pm\cdots\pm z_{2n-1})], \tag{36a}$$

and those of $\mathbf{M}_-$ are

$$(\pm)\exp[\tfrac{1}{2}(\pm z_0\pm z_2\pm z_4\pm\cdots\pm z_{2n-2})]. \tag{36b}$$

To complete the solution of the eigenvalue problem, it is necessary to select the eigenvalues of $\mathbf{M}_+$ belonging to even eigenfunctions, those of $\mathbf{M}_-$ belonging to odd eigenfunctions and to determine the correct sign $(\pm)$ of (36a,b).

In the expressions (36a,b), those eigenvalues with an even number of minus signs in the exponent belong to one of the two subspaces and those with an odd number of minus belong to the other subspace.[6] It is possible to determine from $\mathfrak{M}_\pm$ which subspace goes with the even number of minus signs and which goes with the odd number of minus signs. The procedure is to determine explicitly an orthogonal transformation which carries $\mathfrak{M}$ into its canonical form. Knowing the spin representative associated with the canonical form and whether the orthogonal transformation has determinant $+1$ or -1, one can decide which sign combinations to select in the exponent of (36a,b). Though one can easily find an orthogonal transformation of desired type, the evaluation of its determinant presents difficulties. It is possible, however, to determine uniquely the eigenvalues of $\mathbf{M}$ by a less direct approach.

Equation (2) shows that in that representation $\mathbf{M}$ has all real, non-negative elements. If $\mathbf{M}$ is transformed to the space of even and odd functions, that part of $\mathbf{M}$ belonging to even functions also has non-negative elements. Frobenius[7] and Oldenburger[8] have shown that

[6] See reference 2, pp. 1238, 1239.
[7] S. B. Frobenius, Preuss. Akad. Wiss. 514 (1909).
[8] R. Oldenburger, Duke Math. J. 6, 357 (1940).

if the elements of a matrix are real and non-negative, then the characteristic value with maximum absolute value is real and non-negative.

If we assume that the eigenvalues (36a) with an even number of minus signs belong to the space of even eigenfunctions, then the eigenvalue of $\mathbf{M}$ with the largest absolute value in this space is

$$\max\lambda_+ = (\pm)(2\sinh 2H)^{\frac{1}{2}} c_+ \exp[\tfrac{1}{2}(z_1+z_3+\cdots z_{2n-1})].$$

The value $y_n=\pi$ yields a solution of (32a,b) if n is odd. All other solutions of (32a,b) occur in complex conjugate pairs with $\pm y$ in the range (35). Thus

$$\max\lambda_+ = (\pm)(2\sinh 2H)^{\frac{1}{2}} \times\exp[\tfrac{1}{2}(x_1+x_3+\cdots x_{2n-1})]. \quad (37)$$

We see that Frobenius' theorem is satisfied for the plus sign and the assumption that an even number of minus signs in the exponent gives the desired set of eigenvalues from (36a).

The alternative assumption, that the eigenvalues of (36a) with an odd number of minus signs belong to the space of even functions, leads to a contradiction. Under this assumption, the largest eigenvalue is obtained by choosing all the signs in (36a) positive except the one before the smallest x. By (32a), the smallest x is obtained by taking $|y|$ small. The value $y=0$ is not, however, a solution in the space of even functions, therefore the largest eigenvalue will not be real contrary to Frobenius' theorem.

A similar argument can be applied to the space of odd functions. Though some of the elements of $\mathbf{M}$ are negative in the space of odd basis vectors considered previously, the elements of $\mathbf{M}$ are all non-negative when referred to the system of odd and even basis vectors which are the eigenfunctions of $\mathbf{C}_j$ provided $H'\geq 0$ and $H\geq 0$. With this restriction, Frobenius' theorem can be applied to the odd space. The same arguments as before lead to

$$\max\lambda_- = (\pm)(2\sinh 2H)^{\frac{1}{2}} \times\exp[\tfrac{1}{2}(\pm x_0+x_2+x_4+\cdots+x_{2n-2})]. \quad (38)$$

The proper sign in front is the plus sign. In this case, however, one does not succeed in ruling out either of the possible assumptions regarding the distribution of signs in the exponent of (36b) because $z_0=x_0$ is real. Changing the sign of z_0 does not effect the agreement with Frobenius theorem.

The quantity x_0 is unique in that it is the only x_j that can be zero for finite n. We have $x_0=0$ for $H'=H^*$. The absolute value of dx_0/dT at $H'=H^*$ is not zero; thus if x_0 does not change sign at this point $d(\max\lambda_-)/dT$ will have a discontinuity. A calculation of Z from (4) assuming $x_0\geq 0$ for all T leads to a function which for finite n and m is not analytic in T at the point $H'=H^*$. This is contrary to the definition (1). We define the sign of x_0 by

$$x_0=|x_0| \text{ for } H'>H^*, \quad x_0=-|x_0| \text{ for } H'<H^*. \quad (39)$$

Finally, to select the correct sign before x_0 in (38) one can calculate Z in the limit H', $H\gg 1$. In this limit, $nx_j\to 2H'$ for all j and n. In order that Z calculated from (4) approach the correct limit of (1), namely $Z\to 2e^{nm(H+H')}$, it is necessary that $\max\lambda_+\to\max\lambda_-$. The correct sign in (38) is the upper one.

The eigenvalues of $\mathbf{M}$ are now uniquely determined as

$$\left.\begin{aligned}&(2\sinh 2H)^{\frac{1}{2}} c_+ \exp[\tfrac{1}{2}(\pm z_1\pm z_3\pm\cdots\pm z_{2n-1})]\\ \text{and}\quad&(2\sinh 2H)^{\frac{1}{2}} c_- \exp[\tfrac{1}{2}(\pm z_0\pm z_2\pm\cdots\pm z_{2n-2})]\end{aligned}\right\}, \quad (40)$$

where each expression may have only an even number of minus signs in the exponent.

5. DISCUSSION OF RESULTS

The calculations considered here differ from those of Onsager and Kaufman in two respects. Aside from the fact that the boundary conditions assumed in each case are not the same, the matrix $\mathbf{V}$ of Onsager and Kaufman is that associated with a complete row of the lattice whereas the $\mathbf{M}$ used here is associated with a single point of the lattice. To compare the results of the two calculations one should compare $\mathbf{M}^n$ of this paper with their $\mathbf{V}$. λ^n of this paper corresponds to their λ, which we will refer to here as λ' to avoid confusion. Equation (34) shows that nx_j is equal to γ_j of Onsager and Kaufman in the limit $n\to\infty$. Furthermore, they differ for large n only in order n^{-2}. The nth power of the two largest eigenvalues (37), (38), which contains only x_j, thus differ from the two largest λ' only in order n^{-2}.

A comparison of eigenvalues other than these two is complicated slightly by the fact that most of the λ^n are complex whereas the λ' are real. In general, the λ^n, which occur in complex conjugate pairs, differ from the λ' in absolute value only in order n^{-2}.

The value of the partition function Z for large n and m is accurately expressed in terms of the largest eigenvalues of $\mathbf{M}$. For large temperatures $H'<H^*$, $\max\lambda_+$ is non-degenerate, whereas for $H'>H^*$, $\max\lambda_-$ as $n\to\infty$ and one has a twofold degeneracy of the largest eigenvalues. In neither case do the other eigenvalues give an appreciable contribution to Z. Only in the immediate vicinity of the transition point $H'=H^*$ need they be considered. Here one sees from (32a,b) that if $|y_j|\ll 1$ then $nx_j\ll 1$. At $H'=H^*$ one can, by making n large enough, obtain solutions x_s arbitrarily small. The eigenvalues (37), (38) approach a degeneracy with those eigenvalues in which the sign of an even number of such x_j are changed. As $n\to\infty$, these eigenvalues form a dense sequence of values with $\max\lambda_+$ as their limit.

To complete the comparison of these calculations with those of Onsager and Kaufman, it is necessary only to compare those eigenvalues λ^n, λ' which contribute to Z near the transition point. The complex phase of such λ^{nm} is of order m/n^2. The sum of λ^{nm} and its complex conjugate differ from the corresponding two terms of Onsager and Kaufman only in order m^2/n^4 and in order n^{-2}. If m and n are of comparable size, the par-

tition function of this paper and that of Onsager and Kaufman differ in order n^{-2} at most for all values of T.

Because of the smallness of the discrepancy between the two calculations for $n \gg 1$, a detailed study of these differences would seem of little value. The thermodynamic properties and investigations of order in the lattice have been studied in some detail by Onsager and Kaufman.

A two-dimensional system in which the jth point interacts with the $j+m-1$th in addition to the $j+1$th and $j+n$th can also be treated by the methods given here. In such a model each point interacts with six neighbors. The thermodynamic properties of such a system are now being studied.

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Ferromagnetic Resonance Absorption in Magnetite Single Crystals*†

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The microwave resonance absorption technique, at both 1.25 and 3.3 cm wave-lengths, was used to study the ferromagnetic crystalline anisotropy characteristics and g-factor of magnetite Fe_3O_4. The experiments were performed on single crystals, both synthetic and natural, from room temperature to −195°C. Depending upon the temperature, magnetite single crystals were found to have magnetic anisotropy characteristics similar to those of single crystals of the three ferromagnetic elements. From room temperature to −143°C, they behave like nickel; between −143° and the transition which magnetite is known to undergo at *ca.* −160°C, like iron; and below the transition, somewhat like cobalt. At room temperature, values of $g=2.12$ and K_1 (first-order anisotropy constant) $=-1.10\times10^4$ joule/m^3 (-1.10×10^5 erg/cm^3) were obtained. It was found that below about −90°C the absolute value of K_1 decreases with decreasing temperature, reaching zero at *ca.* −143°C. Between −143° and the transition K_1 is positive and increases with decreasing temperature. The vanishing of crystalline anisotropy at −143°C accounts for the peak in initial permeability found near this temperature. The g-value was found to decrease gradually and monotonically with decreasing temperature. The behavior of magnetite in the resonance experiments below the transition seems to indicate that the magnetic symmetry is uniaxial in this temperature region. This conclusion is consistent with the findings of other investigators. Below the transition the magnetic axis is that [100] direction most nearly parallel to a strong magnetic field applied to the crystal as it is cooled through the transition. At temperatures not far below the transition it is possible to change the magnetic axis from one [100] direction to another by means of a strong magnetic field.

I. INTRODUCTION

THE investigation reported here was part of a program initiated at the Laboratory for Insulation Research to study the fundamental properties of magnetite, as the first step in a longer-range plan to investigate the properties of ferromagnetic semiconductors. Its object was to study magnetite by the microwave resonance technique from room temperature to liquid nitrogen temperature. As will be seen, the microwave resonance absorption experiment is capable of yielding information concerning ferromagnetic crystalline anisotropy. Specifically, it provides one with sufficient information to calculate the anisotropy constants appearing in the energy expression of a ferromagnetic crystal. In addition, it gives a value of the spectroscopic splitting factor, or g-factor, for the material.

II. PROPERTIES OF MAGNETITE

It has been established by Verwey and co-workers[1–3] that magnetite possesses the cubic inverse spinel structure. The explanation proposed[1] for the high electrical conductivity of magnetite at room temperature (10^{-2} ohm cm) is that the distribution of ferrous and ferric ions among the octahedral cation lattice sites is random and fluctuating. That is, one can think of all 16 of these positions as being occupied by ferric ions, with 8 electrons continually changing their position from one site to another.

In a wide range around room temperature, the magnetic properties of magnetite are quite similar to those of nickel. Its saturation magnetization (4.6×10^5 amp/m or 460 c.g.s/cm^3) is about the same as for nickel, and, like nickel, its direction of easy magnetization is the body diagonal [111].

Millar[4] determined the specific heat as a function of temperature, and found an anomalous peak *ca.* 10° wide

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