a rough value of the current amplitude at resonance. We find for the current at resonance

$$I=-\left[2\pi c\left(\frac{\kappa}{\mu}\right)^{\frac{1}{2}}a\right]0.04\cos\left(\frac{3\pi}{2}\xi\right)\cos\omega\tau. \qquad \text{(III-25)}$$

The current is in phase with the impressed electromotive force in the two extreme thirds of the antenna, but out of phase in the middle third. As the current amplitude at the center of the antenna is only some 4 percent of that at first resonance, the second and higher order resonances are evidently of little importance as compared with the first resonance.

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Crystal Statistics. I. A Two-Dimensional Model with an Order-Disorder Transition

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The partition function of a two-dimensional "ferromagnetic" with scalar "spins" (Ising model) is computed rigorously for the case of vanishing field. The eigenwert problem involved in the corresponding computation for a long strip crystal of finite width (n atoms), joined straight to itself around a cylinder, is solved by direct product decomposition; in the special case $n=\infty$ an integral replaces a sum. The choice of different interaction energies ($\pm J$, $\pm J'$) in the (0 1) and (1 0) directions does not complicate the problem. The two-way infinite crystal has an order-disorder transition at a temperature $T=T_c$ given by the condition

$$\sinh(2J/kT_c)\sinh(2J'/kT_c)=1.$$

The energy is a continuous function of T; but the specific heat becomes infinite as $-\log|T-T_c|$. For strips of finite width, the maximum of the specific heat increases linearly with $\log n$. The order-converting dual transformation invented by Kramers and Wannier effects a simple automorphism of the basis of the quaternion algebra which is natural to the problem in hand. In addition to the thermodynamic properties of the massive crystal, the free energy of a (0 1) boundary between areas of opposite order is computed; on this basis the mean ordered length of a strip crystal is

$$(\exp(2J/kT)\tanh(2J'/kT))^n.$$

INTRODUCTION

THE statistical theory of phase changes in solids and liquids involves formidable mathematical problems.

In dealing with transitions of the first order, computation of the partition functions of both phases by successive approximation may be adequate. In such cases it is to be expected that both functions will be analytic functions of the temperature, capable of extension beyond the transition point, so that good methods of approximating the functions may be expected to yield good results for their derivatives as well, and the heat of transition can be obtained from the difference of the latter. In this case, allowing the continuation of at least one phase into its metastable range, the heat of transition, the most appropriate measure of the discontinuity, may be considered to exist over a range of temperatures.

It is quite otherwise with the more subtle transitions which take place without the release of latent heat. These transitions are usually marked by the vanishing of a physical variable, often an asymmetry, which ceases to exist beyond the transition point. By definition, the strongest possible discontinuity involves the specific heat. Experimentally, several types are known. In the $\alpha-\beta$ quartz transition,[1] the specific heat becomes infinite as $(T_c-T)^{-\frac{1}{2}}$; this may be the rule for a great many structural transformations in crystals. On the other hand, supraconductors exhibit a clear-cut finite discontinuity of the specific heat, and the normal state can be continued at will below the transition

[1] H. Moser, Physik. Zeits. **37**, 737 (1936).

point by the application of a magnetic field.[2] Ferromagnetic Curie points[1, 3] and the transition of liquid helium to its suprafluid state[4] are apparently marked by essential singularities of the specific heats; in either case it is difficult to decide whether the specific heat itself or its temperature coefficient becomes infinite. Theoretically, for an ideal Bose gas the temperature coefficient of the specific heat should have a finite discontinuity at the temperature where "Einstein condensation" begins.

In every one of these cases the transition point is marked by a discontinuity which does not exist in the same form at any other temperature; for even when a phase can be continued beyond its normal range of stability, the transition in the extended range involves a finite heat effect.

Whenever the thermodynamic functions have an essential singularity any computation by successive approximation is difficult because the convergence of approximation by analytic functions in such cases is notoriously slow.

When the existing dearth of suitable mathematical methods is considered, it becomes a matter of interest to investigate models, however far removed from natural crystals, which yield to exact computation and exhibit transition points.

It is known that no model which is infinite in one dimension only can have any transition.[5, 6]

The two-dimensional "Ising model," originally intended as a model of a ferromagnetic,[7] is known to be more properly representative of condensation phenomena in the two-dimensional systems formed by the adsorption of gases on the surfaces of crystals.[8] It is known that this model should have a transition.[9] Recently, the transition point has been located by Kramers and Wannier.[10] In the following, the partition function and derived thermodynamic functions will be computed for a rectangular lattice with different interaction constants in two perpendicular directions; this generalization is of some interest and does not add any difficulties.

The similar computation of the partition functions for hexagonal and honeycomb lattices involves but relatively simple additional considerations. A general form of the dual transformation invented by Kramers and Wannier together with a rather obvious "star-triangle" transformation are used in this connection, and the transition points can be computed from the transformations alone. While these were a great help to the discovery of the present results, the logical development of the latter is best relieved of such extraneous topics, and the subject of transformations will be reserved for later communication.

OUTLINE OF METHOD

As shown by Kramers and Wannier,[10] the computation of the partition function can be reduced to an eigenwert problem. This method will be employed in the following, but it will be convenient to emphasize the abstract properties of relatively simple operators rather than their explicit representation by unwieldy matrices.

For an introduction to the language we shall start with the well-known problem of the linear lattice and proceed from that to a rectangular lattice on a finite base. For symmetry we shall wrap the latter on a cylinder, only straight rather than in the screw arrangement preferred by Kramers and Wannier.

The special properties of the operators involved in this problem allow their expansion as linear combinations of the generating basis elements of an algebra which can be decomposed into direct products of quaternion algebras. The representation of the operators in question can be reduced accordingly to a sum of direct products of two-dimensional representations, and the roots of the secular equation for the problem in hand are obtained as products of the roots of certain quadratic equations. To find all the roots requires complete reduction, which is best performed by the explicit construction of a transforming matrix, with valuable by-products of

[2] W. H. Keesom, Zeits. f. tech. Physik **15**, 515 (1934); H. G. Smith and R. O. Wilhelm, Rev. Mod. Phys. **7**, 237 (1935).
[3] H. Klinkhardt, Ann. d. Physik [4], **84**, 167 (1927).
[4] W. H. and A. P. Keesom, Physica **2**, 557 (1935); J. Satterly, Rev. Mod. Phys. **8**, 347 (1938); K. Darrow, *ibid.* **12**, 257 (1940).
[5] E. Montroll, J. Chem. Phys. **9**, 706 (1941).
[6] K. Herzfeld and M. Goeppert-Mayer, J. Chem. Phys. **2**, 38 (1934).
[7] E. Ising, Zeits. f. Physik **31**, 253 (1925).
[8] R. Peierls, Proc. Camb. Phil. Soc. **32**, 471 (1936).
[9] R. Peierls, Proc. Camb. Phil. Soc. **32**, 477 (1936).
[10] H. A. Kramers and G. H. Wannier, Phys. Rev. **60**, 252, 263 (1941).

FIG. 1. Linear crystal model. Spin of entering atom ○ depends statistically on spin of atom in previous end position ●.

identities useful for the computation of averages pertaining to the crystal. This important but formidable undertaking will be reserved for a later communication. It so happens that the representations of maximal dimension, which contain the two largest roots, are identified with ease from simple general properties of the operators and their representative matrices. The largest roots whose eigenvectors satisfy certain special conditions can be found by a moderate elaboration of the procedure; these results will suffice for a qualitative investigation of the spectrum. To determine the thermodynamic properties of the model it suffices to compute the largest root of the secular equation as a function of the temperature.

The passage to the limiting case of an infinite base involves merely the substitution of integrals for sums. The integrals are simplified by elliptic substitutions, whereby the symmetrical parameter of Kramers and Wannier[10] appears in the modulus of the elliptic functions. The modulus equals unity at the "Curie point"; the consequent logarithmic infinity of the specific heat confirms a conjecture made by Kramers and Wannier. Their conjecture regarding the variation of the maximum specific heat with the size of the crystal base is also confirmed.

THE LINEAR ISING MODEL

As an introduction to our subsequent notation we shall consider a one-dimensional model which has been dealt with by many previous authors.[7,10] (See Fig. 1.)

Consider a chain of atoms where each atom (k) possesses an internal coordinate $\mu^{(k)}$ which may take the values ± 1. The interaction energy between each pair of successive atoms depends on whether their internal coordinates are alike or different:

$$u(1,1)=u(-1,-1)=-u(1,-1)=-u(-1,1)=-J,$$

or

$$u(\mu^{(k)},\mu^{(k-1)})=-J\mu^{(k)}\mu^{(k-1)}. \tag{1}$$

The partition function of this one-dimensional crystal equals

$$e^{-F/kT}=Q(T) \tag{2}$$
$$=\sum_{\mu^{(1)},\mu^{(2)},\cdots,\mu^{(N)}=\pm 1}\exp(-\sum_k u(\mu^{(k)},\mu^{(k-1)})/kT).$$

Following Kramers and Wannier,[10] we express this sum in terms of a matrix whose elements are

$$(\mu|\,V\,|\mu')=e^{-u(\mu,\mu')/kT}. \tag{3}$$

Then the summation over $(\mu^{(2)},\cdots,\mu^{(N-1)})$ in (2) is equivalent to matrix multiplication, and we obtain

$$Q(T)=\sum_{\mu 1,\,\mu N}(\mu^{(1)}|\,V^{N-1}\,|\mu^{(N)})=\lambda_m{}^N O(1), \tag{4}$$

where λ_m is the greatest characteristic number of the matrix V. Since all the elements of this matrix are positive, λ_m will be a simple root of the secular equation

$$|\,V-\lambda\,|=0,$$

and the identity

$$\lambda_m\psi_m(\mu)=(V,\psi_m(\mu)) \tag{5}$$

will be satisfied by a function (eigenvector) $\psi_m(\mu)$ which does not change sign.[11] In the present case we have

$$\psi_m(1)=\psi_m(-1)$$
$$\lambda_m=2\cosh(J/kT). \tag{6}$$

It will be convenient to use the abbreviation

$$J/kT=H. \tag{7}$$

The matrix V, written explicitly

$$V=\begin{pmatrix} e^H, & e^{-H} \\ e^{-H}, & e^H \end{pmatrix}, \tag{8}$$

represents an operator on functions $\psi(\mu)$, which has the effect

$$(V,\psi(\mu))=e^H\psi(\mu)+e^{-H}\psi(-\mu). \tag{9}$$

This operator is therefore a function of the "complementary" operator C which replaces μ by $-\mu$

$$(C,\psi(\mu))=\psi(-\mu);\quad C^2=1, \tag{10}$$

[11] S. B. Frobenius, Preuss. Akad. Wiss. pp. 514–518 (1909); R. Oldenberger, Duke Math. J. **6**, 357 (1940). See also E. Montroll, reference 5.

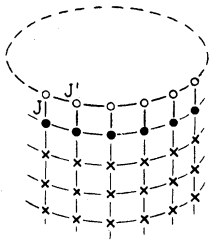


FIG. 2. Cylindrical crystal model. Configuration of added tier—○—○—○— depends on that of tier —●—●—●— in previous marginal position.

and whose eigenfunctions are the (two) different powers of μ

$$(C, 1)=1, \quad (C, \mu)=-\mu, \tag{11}$$

with the characteristic numbers $+1$ and -1, respectively. The linearized expression of V in terms of C is evident from (9), which is now written more compactly

$$V=e^{H}+e^{-H}C. \tag{12}$$

The eigenfunctions of V are of course the same as those of C, given by (11); the corresponding characteristic numbers are

$$\begin{aligned}\lambda_m=\lambda_+&=e^{H}+e^{-H}=2\cosh H\\ \lambda_-&=e^{H}-e^{-H}=2\sinh H.\end{aligned} \tag{13}$$

We shall deal frequently with *products* of many operators of the type (12). It is therefore a matter of great interest to linearize the *logarithm* of such an operator. Following Kramers and Wannier,[10] we introduce the function of H

$$H^*=\tfrac{1}{2}\log\coth H=\tanh^{-1}(e^{-2H}), \tag{14}$$

and obtain

$$V=e^{H}(1+e^{-2H}C)=e^{H}(1+(\tanh H^*)C),$$

which may be written

$$\begin{aligned}V&=(e^{H}/\cosh H^*)\exp(H^*C)\\ &=(2\sinh 2H)^{\frac{1}{2}}\exp(H^*C).\end{aligned} \tag{15}$$

The first, less symmetrical form serves to keep a record of the sign when H is not a positive real number. For example,

$$\begin{aligned}(-H)^*&=H^*\pm\tfrac{1}{2}\pi i\\ \cosh((-H)^*)&=\pm i\sinh H^*.\end{aligned} \tag{16}$$

For reference, we tabulate here the relations given by Kramers and Wannier.

$$\begin{aligned}\sinh 2H\sinh 2H^*&=\cosh 2H\tanh 2H^*\\ &=\tanh 2H\cosh 2H^*=1.\end{aligned} \tag{17}$$

Alternatively, we can express the hyperbolic functions in terms of the gudermannian angle

$$\operatorname{gd} u\equiv 2\tan^{-1}(e^{u})-\tfrac{1}{2}\pi=2\tan^{-1}(\tanh\tfrac{1}{2}u), \tag{18}$$

whereby

$$\begin{aligned}\sinh u\cot(\operatorname{gd} u)&=\coth u\sin(\operatorname{gd} u)\\ &=\cosh u\cos(\operatorname{gd} u)=1.\end{aligned} \tag{19}$$

Then the relation between H and H^* may be written in the form

$$\operatorname{gd} 2H+\operatorname{gd} 2H^*=\tfrac{1}{2}\pi. \tag{20}$$

THE RECTANGULAR ISING MODEL

We consider n parallel chains of the same type as before. We shall build up these chains simultaneously, tier by tier, adding one atom to each chain in one step (see Fig. 2). With the last atom in the jth chain is associated the variable μ_j, capable of the values ± 1. A complete set of values assigned to the n variables describes a configuration $(\mu)=(\mu_1, \cdots, \mu_n)$ of the last tier of atoms. The operator which describes the addition of a new tier with the interaction energy

$$u_1((\mu), (\mu'))=-\sum_{j=1}^{n} J\mu_j\mu_j'=-kTH\sum\mu_j\mu_j' \tag{21}$$

is now

$$\begin{aligned}V_1&=\prod_{j=1}^{n}(e^{H}+e^{-H}C_j)\\ &=(2\sinh 2H)^{n/2}\exp(H^*B),\end{aligned} \tag{22}$$

whereby

$$B\equiv\sum_{j=1}^{n} C_j, \tag{23}$$

and the individual operators $C_1, \cdots, C_n$ have the effect

$$\begin{aligned}&(C_j, \psi(\mu_1, \cdots, \mu_j, \cdots, \mu_n))\\ &\quad=\psi(\mu_1, \cdots, \mu_{j-1}, -\mu_j, \mu_{j+1}, \cdots, \mu_n).\end{aligned} \tag{24}$$

Next, let us assume a similar interaction between adjacent atoms in a tier, only with an independent value J' for the pairwise energy of interaction. For symmetry, let the nth atom be neighbor to the first; then with the convention

that the atoms in a tier are numbered modulo n,

$$\mu_{j+n}=\mu_j,$$

the total tierwise interaction energy will be

$$u_2(\mu_1, \cdots, \mu_n) = -J'\sum_{j=1}^{n}\mu_j\mu_{j+1}=-kTH'\sum_{j=1}^{n}\mu_j\mu_{j+1}. \quad (25)$$

The effect of this interaction is simply to multiply the general term of the partition function, represented by one of the 2^n vector components $\psi(\mu_1, \cdots, \mu_n)$, by the appropriate factor $\exp(-u_2(\mu_1, \cdots, \mu_n)/kT)$; the corresponding operator V_2 has a diagonal matrix in this representation. It can be constructed from the simple operators $s_1, \cdots, s_n$ which multiply ψ by its first, $\cdots$, nth argument, as follows

$$(s_j, \psi(\mu_1, \cdots, \mu_n))=\mu_j\psi(\mu_1, \cdots, \mu_n) \quad (26)$$

$$A=\sum_{j=1}^{n}s_js_{j+1}, \quad (27)$$

$$V_2=\exp(H'A). \quad (28)$$

We now imagine that we build the crystal in alternate steps. We first add a new tier of atoms (see Fig. 3), next introduce interaction among atoms in the same tier, after that we add another tier, etc. The alternate modifications of the partition function are represented by the product

$$\cdots V_2\ V_1\ V_2\ V_1\ V_2\ V_1$$

with alternating factors; the addition of one tier of atoms with interaction both ways is represented by $(V_2V_1)=V$. The eigenwert problem which yields the partition function of the crystal is accordingly

$$\lambda\psi=(V, \psi)=(V_2V_1, \psi)$$
$$=(2\sinh 2H)^{n/2}(\exp(H'A)\exp(H^*B), \psi). \quad (29)$$

Viz., in the more explicit matrix notation used by previous authors[12]

$$\lambda\psi(\mu_1\cdots\mu_n)=\exp\left(H'\sum_{1}^{n}\mu_j\mu_{j+1}\right)$$
$$\times\sum_{\mu_1'\cdots\mu_n'=\pm1}\exp\left(H\sum_{1}^{n}\mu_j\mu_j'\right)\psi(\mu_1'\cdots\mu_n').$$

[12] See H. A. Kramers and G. H. Wannier (reference 10). E. Montroll (reference 5); E. N. Lassettre and J. P. Howe, J. Chem. Phys. **9**, 747 (1941).

This 2^n-dimensional problem we shall reduce to certain sets of 2-dimensional problems. So far, we have expressed A and B rather simply by the generating elements $s_1, C_1, \cdots, s_n, C_n$ of a certain abstract algebra, which is easily recognized as a direct product of n quaternion algebras. However, the expansion (27) of A is not linear. Following a preliminary study of the basis group, we shall therefore construct a new basis for a part of the present algebra, which allows linear expansions of both A and B in terms of its generating elements.

QUATERNION ALGEBRA

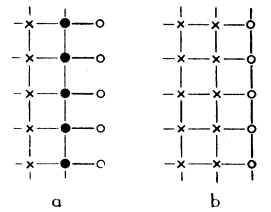
We have introduced two sets of linear operators $s_1, \cdots, s_n$ and $C_1, \cdots, C_n$ by the definitions

$$\begin{aligned}(s_j, \psi(\mu_1, \cdots, \mu_j, \cdots, \mu_n)) &= \mu_j\psi(\mu_1, \cdots, \mu_j, \cdots, \mu_n),\\ (C_j, \psi(\mu_1, \cdots, \mu_j, \cdots, \mu_n)) &= \psi(\mu_1, \cdots, -\mu_j, \cdots, \mu_n).\end{aligned} \quad (30)$$

We shall see that the group generated by these operators forms a complete basis for the algebra of linear operators in the 2^n-dimensional vector space of the functions $\psi(\mu_1, \cdots, \mu_n)$. Their abstract properties are

$$\begin{aligned}&s_j^2=C_j^2=1, \quad s_jC_j=-C_js_j;\\ &s_js_k=s_ks_j, \quad C_jC_k=C_kC_j;\\ &s_jC_k=C_ks_j; \quad (j\neq k).\end{aligned} \quad (31)$$

The algebra based on one of the subgroups $(1, s_j, C_j, s_jC_j)$ is a simple quaternion algebra. The group of its basis elements includes $(-1, -s_j, -C_j, C_js_j)$ as well; but this completion of the group adds no new independent element for the purpose of constructing a basis. If we disregard



a b

FIG. 3. Two-step extension of a two-dimensional crystal. (a) A new tier of atoms ○ is added (V_1); their configuration depends on that of atoms ● in previous marginal position. (b) Interaction energy between marginal atoms ○ is introduced (V_2), which modifies the distribution of configurations in this tier of atoms.

the sign, each element is its own inverse. Except for the invariant element (-1) and the unit proper, each element together with its negative constitutes a class. This algebra has just one irreducible representation

$$\mathbf{D}_2(1)=\begin{pmatrix}1&0\\0&1\end{pmatrix};\quad \mathbf{D}_2(s_j)=\begin{pmatrix}1&0\\0&-1\end{pmatrix};$$

$$\mathbf{D}_2(C_j)=\begin{pmatrix}0&1\\1&0\end{pmatrix};\quad \mathbf{D}_2(s_jC_j)=\begin{pmatrix}0&1\\-1&0\end{pmatrix}.$$

Our algebra of operators in 2^n-dimensional space can be described accordingly as the direct product of n simple quaternion algebras, which is still referred to as a (general) quaternion algebra. Each one of its 4^n independent basis elements can be expressed uniquely as a product of n factors, one from each set $(1, s_j, C_j, s_jC_j)$. Still, each element furnishes its own inverse and, except for (-1) and the unit, each element with its negative constitutes a class, which immediately characterizes all possible representations of the algebra: *The characters of all basis elements with the sole exception of the unit must vanish.* This of course is a consequence of the direct product construction. Another is the recognition that the algebra has only one irreducible representation

$$\mathbf{D}_2\times\mathbf{D}_2\times\cdots\times\mathbf{D}_2=\mathbf{D}_{2^n}$$

which is of 2^n dimensions; our definitions (30) describe an explicit version of it.

With the customary restriction that the elements of the basis group are to be represented by unitary matrices, the representations of the 4^n independent basis elements must be orthogonal to each other (in the hermitian sense) on the 2^{2n} (or more) matrix elements as a vector basis. For the vector product in question is nothing but

$$\sum_{r,s=1}^{2^n}\mathbf{D}(Q_1)_{rs}\overline{\mathbf{D}}(Q_2)_{rs}=\mathrm{Tr.}\,(\mathbf{D}(Q_1Q_2^{-1}))=\mathrm{Tr.}\,(\mathbf{D}(Q_3)),$$

and if Q_1 and Q_2 are independent elements of the basis group, then their quotient Q_3 is an element different from the unit and (-1), so that its character vanishes.

Since orthogonality guarantees linear independence, the irreducible 2^n-dimensional representation of our 4^n independent basis elements will suffice for the construction of any $2^n\times 2^n$ matrix by linear combination; *our quaternion algebra is equivalent to the complete matrix algebra of 2^n dimensions.* The choice between the two forms is a matter of convenience; the quaternion description seems more natural to the problem in hand. One of the main results obtained by Kramers and Wannier will be derived below; the comparison with their derivation is instructive.

In the following, the entire basis group will not be needed. Since our operator A involves only products of pairs of the generating elements $s_1, \cdots, s_n$ and B does not involve any of these but only $C_1, \cdots, C_n$, we shall have to deal only with that subgroup of the basis which consists of elements containing an *even* number of factors s_j. This "even" subgroup, which comprises half the previous basis, may be characterized equally well by the observation that it consists of those basis elements which commute with the operator

$$C=C_1C_2\cdots C_n \tag{32}$$

which reverses all spins at once

$$(C,\psi(\mu_1,\cdots,\mu_n))=\psi(-\mu_1,\cdots,-\mu_n). \tag{32a}$$

The representation (30) is now reducible because the 2^{n-1} *even* functions satisfying

$$(C,\psi)=\psi$$

are transformed among themselves as are the *odd* functions satisfying

$$(C,\psi)=-\psi.$$

The corresponding algebras are both of the same type as before, with $(n-1)$ pairs of generating elements

$$s_1s_n, s_2s_n, \cdots, s_{n-1}s_n;\quad C_1, C_2, \cdots, C_{n-1}$$

and either algebra is equivalent to the complete matrix algebra of 2^{n-1} dimensions. The previously independent operator C_n is now expressible by the others because either $C=1$ or $C=-1$, according to whether we are dealing with even or odd functions. This choice of sign determines the only difference between the two versions of the algebra in question. Moreover, the operator

$$A=\sum_{j=1}^{n}s_js_{j+1}$$

is the same in both versions, but obviously

$$B=\sum_{j=1}^{n} C_j$$

is not; here the interpretation of C_n makes a difference.

The arbitrary elimination of one of the sets of operators which enter symmetrically into the problem causes much inconvenience. The symmetry can be retained if we start with the two series of operators

$$s_1s_2,\ s_2s_3,\ \cdots,\ s_ns_1;\quad C_1,\ C_2,\ \cdots,\ C_n \tag{33}$$

required to satisfy the identities

$$s_1s_2s_2s_3\cdots s_ns_1=s_1^2s_2^2\cdots s_n^2=1$$

$$C_1C_2\cdots C_n=C=\begin{cases}1; & \text{(even functions)}\\ -1; & \text{(odd functions).}\end{cases} \tag{34}$$

The commutation rules are simply described when the two sets are arranged in the interlacing cyclic sequence

$$s_ns_1,\ C_1,\ s_1s_2,\ C_2,\ \cdots,\ s_{n-1}s_n,\ C_n,\ (s_ns_1,\ \cdots). \tag{35}$$

Here each element anticommutes with its neighbors and commutes with all other elements in the sequence.

Dual Transformation

The fundamental algebraic reason for the dual relation found by Kramers and Wannier is now readily recognized: *In the representation which belongs to even functions*, the two sets (33) are alike because the starting point of the sequence (35) is immaterial. Neither does it matter if the sequence is reversed, so that the general rules of computation remain unchanged if each member of the sequence (35) is replaced by the corresponding member of the sequence

$$C_k,\ s_ks_{k\pm1},\ C_{k\pm1},\ s_{k\pm1}s_{k\pm2},\ \cdots.$$

Accordingly, the correspondence

$$s_js_{j+1}\rightarrow C_{k\pm j},\quad C_j\rightarrow s_{k\pm(j-1)}s_{k\pm j} \tag{36}$$

describes an automorphism of the whole algebra. Under this automorphism we have in particular

$$A\rightarrow B$$
$$B\rightarrow A$$

or, compactly

$$f(A, B)\rightarrow f(B, A),$$

all in the algebra of even functions. Similarity can be inferred from the additional observation that the characters of all representations are determined by the commutation rules, or equally well from the theorem that every automorphism of a complete matrix algebra is an internal automorphism. When we return to our original mixed algebra of even and odd functions, our result takes the form

$$(1+C)f(A, B)\sim(1+C)f(B, A). \tag{37}$$

Application to the operator V given by (29) shows that the two operators

$$(\sinh 2H)^{-n/2}(1+C)\,V(H', H)$$
$$=2^{-n/2}(1+C)\exp(H'A)\exp(H^*B),$$
$$(\sinh 2H')^{n/2}(1+C)\,V'(H^*, H'^*)$$
$$=2^{-n/2}(1+C)\exp(H'B)\exp(H^*A)$$

are similar, so that the part of the spectrum of $V(H^*, H'^*)$ which belongs to even functions can be obtained from the corresponding part of the spectrum of $V(H', H)$ by the relation

$$\lambda_+(H^*, H'^*)$$
$$=(\sinh 2H\sinh 2H')^{-n/2}\lambda_+(H', H). \tag{38}$$

This result applies in particular to the largest characteristic numbers of the operators in question because both can be represented by matrices with all positive elements so that, by Frobenius' theorem,[11] the corresponding eigenvectors cannot be odd.

In the "screw" construction of a crystal preferred by Kramers and Wannier,[10] the addition of one atom is accomplished by the operator ($\mathfrak{M}$ in their notation)

$$\exp(Hs_{n-1}s_n)(\sinh 2H)^{\frac{1}{2}}\exp(H^*C_n)T$$
$$=(\sinh 2H)^{\frac{1}{2}}\exp(Hs_{n-1}s_n)T\exp(H^*C_1),$$

where T is a permutation operator which turns the screw through the angle $2\pi/n$. They indicate in explicit matrix form a transformation which effects one of the automorphisms (36), namely,

$$s_js_{j+1}\rightarrow C_{n-j},\quad C_j\rightarrow s_{n-j+1}s_{n-j}$$

whereby naturally

$$T\rightarrow T^{-1}.$$

The equivalent of (38) follows. In consequence, if the crystal is disordered at high temperatures (small H), a transition must occur at the temperature where the equality

$$H=H^*=\tfrac{1}{2}\log\cot\pi/8 \tag{39a}$$

is satisfied.

Unfortunately, our simplified derivation fails to exhibit one of the most important properties of the "dual" transformation: When applied to large two-dimensional (∞^2) crystal models, it *always* converts order into disorder and vice versa; this result is readily obtained by detailed inspection of the matrix representation. The consequent determination of the transition point for the rectangular crystal by the generalization of (39a)

$$H'=H^*;\quad (kT=kT_c) \tag{39b}$$

will be verified in the following by other means.

On the other hand, the given results are still but special applications of a transformation which applies to all orientable graphs, not just rectangular nets. Except for its "order-converting" property, this transformation is best obtained and discussed in simple topological terms. The properties of the "dual" and certain other transformations will be given due attention in a separate treatise; it would be too much of a digression to carry the subject further at this point.

Fundamental Vector Systems

We shall give brief consideration to the vector basis of our quaternion algebra, as described by the operator formulation (30). The systems of eigenvector which belong to the two sets of operators $(s_1, \cdots, s_n)$ and $(C_1, \cdots, C_n)$ are easily identified. The representations (30) of the former are already diagonal, so that their eigenvectors are δ functions

$$(s_j,\ \delta(\mu_1-\mu_1',\ \cdots,\ \mu_j-\mu_j',\ \cdots,\ \mu_n-\mu_n'))$$
$$=\mu_j'\delta(\mu_1-\mu_1',\ \cdots,\ \mu_j-\mu_j',\ \cdots,\ \mu_n-\mu_n'). \tag{40}$$

The eigenvectors of $(C_1, \cdots, C_n)$ are the different products of $\mu_1, \cdots, \mu_n$, with the normalizing factor $2^{-n/2}$

$$(C_j,\ (\mu_1{}^{\nu_1}\cdots\mu_n{}^{\nu_n}))=(-)^{\nu_j}(\mu_1{}^{\nu_1}\cdots\mu_n{}^{\nu_n}). \tag{41}$$

The explicit representation of a transformation which leads from one of these systems to the other is obtained from the expansion of the identity

$$\delta(\mu_1-\mu_1',\ \cdots,\ \mu_n-\mu_n')$$
$$=2^{-n}(1+\mu_1'\mu_1)\cdots(1+\mu_n'\mu_n). \tag{42}$$

This product description of a δ function is often more convenient. The two systems (40) and (41) yield diagonal representations of the operators A and B, respectively. The construction of the latter is a little simpler. With a slight variation of the notation we find

$$(B,\ (\mu_{j_1}\mu_{j_2}\cdots\mu_{j_k}))=(n-2k)(\mu_{j_1}\mu_{j_2}\cdots\mu_{j_k}), \tag{43a}$$

so that any homogeneous function of $(\mu_1, \cdots, \mu_n)$ is an eigenvector of B. With no repeated factors allowed, the number of independent homogeneous functions of degree k is the binomial coefficient $\binom{n}{k}$. Accordingly, the secular polynomial is

$$|B-\lambda|\equiv\prod_{k=0}^{n}(n-2k-\lambda)^{\binom{n}{k}}. \tag{43b}$$

Whereas B measures the degree of a function $\psi(\mu_1, \cdots, \mu_n)$, the operator A simply counts alternations of sign in the configuration $(\mu_1, \cdots, \mu_n)$. The analog of (43a) is now

$$\left(A,\ \left(\prod_{1}^{j_1}(1+\mu_j)\prod_{j_1+1}^{j_2}(1-\mu_j)\cdots\prod_{j_{2k}+1}^{n}(1+\mu_j)\right)\right)$$
$$=(n-4k)\left(\prod_{1}^{j_1}(1+\mu_j)\prod_{j_1+1}^{j_2}(1-\mu_j)\cdots\right.$$
$$\left.\times\prod_{j_{2k}+1}^{n}(1+\mu_j)\right). \tag{44a}$$

The alternations of sign are located arbitrarily behind $j_1, j_2, \cdots j_{2k}$; but their total number must be even $=2k$. On the other hand, the result (44a) is equally valid when μ_j is replaced throughout by $-\mu_j$; so that the spectrum of A repeats in duplicate that part of the spectrum of B which belongs to even functions, and its secular polynomial is

$$|A-\lambda|\equiv\prod_{k=0}^{[n/2]}(n-4k-\lambda)^{2\binom{n}{2k}}. \tag{44b}$$

By an obvious transformation, one-half of the

paired characteristic numbers of A may be assigned to even functions and the other, identical half to odd functions. We note again that the three operators

$$(1-C)A\sim(1+C)A\sim(1+C)B$$

are similar, whereas $(1-C)B$ has a different structure.

Some Important Elements of the Basis

As a preliminary to the simultaneous reduction of the representation of the operators A and B, we shall consider certain elements of the basis group which will recur frequently in the process and introduce a special notation for them. We have already encountered

$$P_{aa}=-C_a,\quad P_{a,a+1}=s_as_{a+1}.$$

In general we define P_{ab} as the product

$$P_{ab}=s_aC_{a+1}C_{a+2}\cdots C_{b-1}s_b;\qquad (a,b=1,2,\cdots,2n). \quad (45)$$

These operators are elements of the "even" basis and commute with C. They satisfy the recurrence formula

$$P_{a,b+1}=P_{ab}P_{bb}P_{b,b+1}=P_{ab}s_bC_bs_{b+1}. \quad (45a)$$

The period of this recurrence formula is $2n$; increasing either index by n has the effect of a multiplication by $(-C)$

$$P_{a,b+n}=P_{a+n,b}=-CP_{ab}=-P_{ab}C. \quad (46)$$

The product (45) obviously may be written in reverse order when $(b-a)\leqq n$, and by (46), this result is easily extended to all (a,b). Accordingly,

$$P_{ab}^2=s_aC_{a+1}\cdots C_{b-1}s_bs_bC_{b-1}\cdots C_{a+1}s_a=1. \quad (47)$$

More generally, we thus obtain the "rule of the wild index"

$$P_{ac}P_{bc}=P_{ad}P_{bd},\quad P_{ac}P_{ad}=P_{bc}P_{bd}. \quad (48)$$

The analogous result for indices congruent $(\mathrm{mod}=n)$ is obtained immediately by combination with (46)

$$\begin{aligned}&P_{ac}P_{b,c+n}=P_{ad}P_{b,d+n}=P_{ad}P_{b+n,d},\\&P_{ac}P_{a+n,d}=P_{bc}P_{b+n,d}=P_{bc}P_{b,d+n}.\end{aligned} \quad (49)$$

While the period of the recurrence formula (45a) is $2n$, it is evident from (46) that the period of the commutation rules will be just n; for the factor C commutes with all the operators P_{ab}. For this reason we shall need a modified Kronecker symbol with the period n, as follows

$$D(0)=D(n)=1,\quad D(m)\sin(m\pi/n)=0. \quad (50)$$

Indices which differ by 0 or n $(\mathrm{mod}=2n)$ will be called *congruent*; (in the former case we call them equal). Only the congruence of *corresponding* indices matters; no important identity results from the accident that a front index coincides with a rear index. The distinction between front and rear indices represents the distinction between the opposite directions of rotation (1, 2, 3, $\cdots$, n) and (1, n, $n-1$, $\cdots$, 2) around the base of the "crystal."

The effect of simultaneous congruence is evident from (47) together with (46); one obtains either the unit (1) or the invariant basis element $(-C)$. More generally, a product of the form

$$P_{aa'}P_{bb'}\cdots P_{kk'}$$

with any number of factors equals one of the invariant elements ±1, $\pm C$ if both front and rear indices congruent to each of the possible values 1, 2, $\cdots$, n occur an even number (0, 2, 4, $\cdots$) of times. This rule can be obtained from (48) by simple manipulation; compare the derivation of exchange rules below. In addition, thanks to the relation

$$P_{11}P_{22}\cdots P_{nn}=(-)^nC_1C_2\cdots C_n=(-)^nC, \quad (51)$$

an invariant element also results if both front and rear indices congruent to each of the numbers 1, 2, $\cdots$, n occur an *odd* number of times. A count of the group elements shows that there can be no further identities of this sort; accordingly, if a product satisfies neither of the given conditions, it must be a basis element different from ±1 and $\pm C$.

The commutation rules for the operators P_{ab} can be broken up into rules which govern the exchange of indices between adjacent factors in a product. These in turn can be obtained by the rule of the wild index from the commutation rules which involve $P_{aa}=-C_a$. We first consider the product

$$P_{ab}P_{bb}=-P_{ab}C_b=-s_aC_{a+1}\cdots C_{b-1}s_bC_b.$$

When $a \equiv b$, the commutative character of the multiplication is trivial. Otherwise, there is only one factor s_b in P_{ab}; so that this operator anticommutes with $C_b = -P_{bb}$. Accordingly,

$$P_{ab}P_{bb} + (-)^{D(a-b)}P_{bb}P_{ab} = 0.$$

In view of (48) this may be written equally well

$$P_{ac}P_{bc} + (-)^{D(a-b)}P_{bc}P_{ac} = 0.$$

However, the result does not depend on the presence of a wild index, because

$$P_{ac}P_{bd} = P_{ac}P_{ad}P_{ad}P_{bd} = P_{bc}P_{bd}P_{ad}P_{bd} = -(-)^{D(a-b)}P_{bc}P_{ad}P_{bd}^2.$$

The same reasoning applies to the exchange of rear indices, and we obtain the general rule

$$P_{ac}P_{bd} = -(-)^{D(a-b)}P_{bc}P_{ad} = -(-)^{D(c-d)}P_{ad}P_{bc} = (-)^{D(a-b)+D(c-d)}P_{bd}P_{ac}. \quad (52)$$

Accordingly, the exchange of indices between adjacent factors in a product takes place with change of sign unless the trivial exchange of congruent (wild) indices is involved.

The product $P_{ac}P_{bd}$ is seen to be commutative when neither $(a-b)$ nor $(c-d)$ divides n, and in the trivial case when both do. When one and only one congruence exists, the factors anticommute.

For future reference we give here the direct operational definition of P_{ab}. In the case

$$\cot(a-\tfrac{1}{2})\pi/n > \cot(b-\tfrac{1}{2})\pi/n$$

we have

$$(P_{ab}, \psi(\mu_1, \cdots, \mu_n)) = \mu_a\mu_b\psi(\mu_1, \cdots, \mu_a, -\mu_{a+1}, \cdots, -\mu_{b-1}, \mu_b, \cdots, \mu_n); \quad (53a)$$
$$(\sin((b-a-\tfrac{1}{2})\pi/n) > 0)$$

$$(P_{ab}, \psi(\mu_1, \cdots, \mu_n)) = -\mu_a\mu_b\psi(-\mu_1, \cdots, -\mu_a, \mu_{a+1}, \cdots, \mu_{b-1}, -\mu_b, \cdots, -\mu_n); \quad (53b)$$
$$(\sin((b-a-\tfrac{1}{2})\pi/n) < 0).$$

When $\cot(a-\tfrac{1}{2})\pi/n \leqq \cot(b-\tfrac{1}{2})\pi/n$, substantially the same formulas apply, only the changes of sign are arranged $(-\mu_1, \cdots, -\mu_{b-1}, \mu_b, \cdots, \mu_a, -\mu_{a+1}, \cdots, -\mu_n)$ in the case (a) and $(\mu_1, \cdots, \mu_{b-1}, -\mu_b, \cdots, -\mu_a, \mu_{a+1}, \cdots, \mu_n)$ in the case (b).

The given formulas describe the effect of P_{ab} in terms of the vector basis (40). The effect of this same operator on a vector which belongs to the fundamental system (41) can be described conveniently with the aid of functions which introduce a change of sign once in a period $(1, 2, \cdots, n)$. Individually, these functions have the period $2n$. We shall use the standard notation

$$\operatorname{sgn} x = \begin{cases} -1; & x<0 \\ 0; & x=0 \\ 1; & x>0. \end{cases}$$

Then the function

$$\operatorname{sgn}(\sin(j\pi/n))$$

changes sign at $j=0$ and $j=n$ and vanishes for these values of j, while the function

$$\operatorname{sgn}(\sin(j-\tfrac{1}{2})\pi/n)$$

has everywhere the absolute value 1, with changes of sign between 0 and 1, and between n and $n+1$. With this notation we obtain

$$(P_{ab}, \mu_{j_1}\mu_{j_2}\cdots\mu_{j_k}) = \operatorname{sgn}[\sin((b-a-\tfrac{1}{2})\pi/n) \times \prod_{h=1}^{k} (\sin(j_h-a-\tfrac{1}{2})\pi/n \sin(j_h-b+\tfrac{1}{2})\pi/n)] \times \mu_a\mu_b\mu_{j_1}\cdots\mu_{j_k}. \quad (54)$$

This formula can be verified by direct count of the sign changes caused by the operator

$$C_{a+1}C_{a+2}\cdots C_{b-1}$$

acting on each factor of the product

$$\mu_b\mu_{j_1}\mu_{j_2}\cdots\mu_{j_k}.$$

THE BASIS OF A REDUCED REPRESENTATION

Some Important Commutators

The operators

$$A = \sum_1^n s_j s_{j+1} = \sum_1^n P_{a,a+1}, \quad B = \sum_1^n C_j = -\sum_1^n P_{aa}$$

are invariant against the dihedral (rotation-reflection) group of transformations

$$\mu_j \rightarrow \mu_{k\pm j}; \quad (j=1, 2, \cdots, n). \quad (55)$$

From the operators P_{ab} we can form $2n$ linear combinations which exhibit the same symmetry,

most simply as follows:

$$A_m=\sum_{a=1}^{n} P_{a,a+m}, \tag{56}$$

whereby

$$A_0=-B, \quad A_1=A. \tag{56a}$$

In view of (46) we have

$$A_{m+n}=-CA_m=-A_mC. \tag{57}$$

From the commutators

$$[P_{ac}, P_{bd}]=P_{ac}P_{bd}-P_{bd}P_{ac}$$

which vanish unless exactly one congruence between the indices is satisfied, we can form $n-1$ independent linear combinations of dihedral symmetry, which may be written most compactly

$$G_m=\tfrac{1}{4}\sum_{a=1}^{n}([P_{ax}, P_{a+m,x}]-[P_{xa}, P_{x,a+m}])$$
$$=\tfrac{1}{2}\sum_{a=1}^{n}(P_{ax}P_{a+m,x}-P_{xa}P_{x,a+m}). \tag{58}$$

While the definition of G_1, G_2, $\cdots$ will be extended conventionally to the complete period $m=1, 2, \cdots, 2n$, they satisfy the identities

$$G_{-m}=-G_m; \quad G_0=G_n=0 \tag{58a}$$

so that there are only $n-1$ independent operators included in the set. The analog of (57)

$$G_{m+n}=-CG_m=-G_mC \tag{59}$$

is valid. The commutators of $A_1, A_2, \cdots, A_{2n}$ with each other necessarily can be expressed in terms of the set (58). By definition

$$[A_m, A_m]=0.$$

By (57) we have also

$$[A_m, A_{m+n}]=0.$$

If we exclude these trivial cases, the congruences

$$a\equiv b; \quad a+k\equiv b+m$$

will not be satisfied simultaneously when we compute

$$[A_k, A_m]=\sum_{a,b=1}^{n}[P_{a,a+k}, P_{b,b+m}]$$
$$=\sum_{c=1}^{n}[P_{xc}, P_{x,c+m-k}]+\sum_{a=1}^{n}[P_{ax}, P_{a-m+k,x}]$$

whence

$$[A_k, A_m]=4G_{k-m}, \tag{60}$$

With the convention (58a) this is also valid in the trivial case $k\equiv m$. Conversely, the commutators of $A_1, A_2, \cdots, A_{2n}$ with their own commutators $G_1, G_2, \cdots, G_{n-1}$ can be expressed in terms of the former as follows:

$$2[G_m, A_k]=\sum_{a,b=1}^{n}([P_{ax}P_{a+m,x}, P_{b,b+k}]$$
$$-[P_{xa}P_{x,a+m}, P_{b-k,b}]).$$

Again if we exclude the trivial case $m\equiv 0$, the congruences $b\equiv a$, $b\equiv a+m$ will not be satisfied simultaneously. Hence,

$$2[G_m, A_k]=\sum_{a=1}^{n}([P_{ax}P_{a+m,x}, P_{a,a+k}]$$
$$+[P_{ax}P_{a+m,x}, P_{a+m,a+k+m}]$$
$$-[P_{xa}P_{x,a+m}, P_{a-k,a}]$$
$$-[P_{xa}P_{x,a+m}, P_{a-k+m,a+m}]).$$

Here

$$[P_{ax}P_{a+m,x}, P_{a,a+k}]=-2P_{a,a+k}P_{ax}P_{a+m,x}$$
$$=-2P_{a,a+k}P_{a,a+k}P_{a+m,a+k}=-2P_{a+m,a+k},$$

$$[P_{ax}P_{a+m,x}, P_{a+m,a+k+m}]$$
$$=2P_{ax}P_{a+m,x}P_{a+m,a+k+m}=2P_{a,a+k+m},$$

etc., and we obtain

$$2[G_m, A_k]=\sum_{a=1}^{n}(-2P_{a+m,a+k}+2P_{a,a+k+m}$$
$$+2P_{a-k,a+m}-2P_{a-k+m,a})$$
$$=\sum_{a=1}^{n}(4P_{a,a+k+m}-4P_{a,a+k-m}),$$

or, simply

$$[G_m, A_k]=2A_{k+m}-2A_{k-m} \tag{61}$$

which is also valid in the trivial case $m\equiv 0$. It is easily shown from (60) and (61) that the commutators $G_1, \cdots, G_{n-1}$ commute with each other. We have generally

$$[G_m, [A_k, A_0]]=[[G_m, A_k], A_0]+[A_k, [G_m, A_0]].$$

Using this together with (60) and (61) we find

$$[G_m, G_k]=[(2A_{k+m}-2A_{k-m}), A_0]$$
$$+[A_k, (2A_m-2A_{-m})]$$
$$=8G_{k+m}-8G_{k-m}$$
$$+8G_{k-m}-8G_{k+m}=0. \tag{61a}$$

A Set of Generating Basis Elements

The commutation rules (60) and (61) suggest the introduction of the operators $X_0, X_1, \cdots, X_n, Y_1, \cdots, Y_{n-1}, Z_1, \cdots, Z_{n-1}$ defined as follows:

$$X_r=(4n)^{-1}\sum_{a,b=1}^{2n}\cos((a-b)r\pi/n)P_{ab},$$

$$Y_r=(4n)^{-1}\sum_{a,b=1}^{2n}\sin((a-b)r\pi/n)P_{ab}, \tag{62}$$

$$Z_r=(-i/8n)\sum_{a,b=1}^{2n}\sin((a-b)r\pi/n)\times(P_{ax}P_{bx}-P_{xa}P_{xb}).$$

Again these definitions will apply conventionally for the entire period $r=1, 2, \cdots, 2n$, whereby

$$\begin{aligned}&X_{-r}=X_r,\\ &Y_{-r}=-Y_r;\quad Y_0=Y_n=0,\\ &Z_{-r}=-Z_r;\quad Z_0=Z_n=0.\end{aligned} \tag{62a}$$

Comparison of (62) with (56) and (58) yields directly

$$\begin{aligned}X_r&=(2n)^{-1}\sum_{m=1}^{2n}\cos(mr\pi/n)A_m,\\ Y_r&=-(2n)^{-1}\sum_{m=1}^{2n}\sin(mr\pi/n)A_m,\\ Z_r&=(i/2n)\sum_{m=1}^{2n}\sin(mr\pi/n)G_m.\end{aligned} \tag{63a}$$

Conversely, from the orthogonal properties of the coefficients

$$\begin{aligned}A_m&=\sum_{r=1}^{2n}(X_r\cos(mr\pi/n)-Y_r\sin(mr\pi/n)),\\ G_m&=-i\sum_{r=1}^{2n}Z_r\sin(mr\pi/n).\end{aligned} \tag{63b}$$

In particular, A and B admit the expansions

$$\begin{aligned}B=-A_0&=-\sum_1^{2n}X_r=-X_0-2X_1\\ &\quad-\cdots-2X_{n-1}-X_n,\\ A=A_1&=\sum_1^{2n}(X_r\cos(r\pi/n)-Y_r\sin(r\pi/n))\\ &=X_0+2(X_1\cos(\pi/n)\\ &\quad-Y_1\sin(\pi/n))+\cdots\\ &\quad+2(X_{n-1}\cos((n-1)\pi/n)\\ &\quad-Y_{n-1}\sin((n-1)\pi/n))-X_n.\end{aligned} \tag{63c}$$

Conversely, the operators (62) can be constructed from A and B by means of (60), (61), and (63a).

The relations (57) and (59) now become

$$\begin{aligned}(1+(-)^rC)X_r&=(1+(-)^rC)Y_r\\ &=(1+(-)^rC)Z_r=0\end{aligned} \tag{64}$$

so that the operators (62) belong to the algebra of even functions when r is odd, and vice versa; they annihilate even functions for even r and odd functions for odd r. We could deal with each set independently, but the two have many properties in common, and it is often convenient to keep them together.

The commutation rules for the operators (62) are easily obtained from (60) and (61). Thanks to the orthogonal properties of the trigonometric coefficients, we find

$$\begin{aligned}&[X_r, X_s]=[Y_r, Y_s]=[Z_r, Z_s]=0,\\ &[X_r, Y_s]=[Y_r, Z_s]=[Z_r, X_s]=0;\\ &\qquad\cos(r\pi/n)\neq\cos(s\pi/n).\end{aligned} \tag{65a}$$

The only commutators which do not vanish are

$$\begin{aligned}&[X_r, Y_r]=-2iZ_r,\\ &[Y_r, Z_r]=-2iX_r,\quad (r=1, 2, \cdots, n-1)\\ &[Z_r, X_r]=-2iY_r.\end{aligned} \tag{65b}$$

We shall show next that the operators (X_r, Y_r, Z_r), which commute with the members of other sets (X_s, Y_s, Z_s), anticommute among themselves. For this purpose we compute

$$(X_r+iY_r)^2=(4n)^{-2}\sum_{a,b=1}^{2n}e^{(a+b-c-d)r\pi i/n}P_{ac}P_{bd}$$

by the definition (62). In the given expansion we may interchange (a, b) and (c, d) independently without disturbing the coefficient. Taking the mean of the four alternatives we obtain

$$(8n)^{-2}\sum_{a,b=1}^{2n}e^{(a+b-c-d)r\pi i/n}\times(P_{ac}P_{bd}+P_{ad}P_{bc}+P_{bc}P_{ad}+P_{bd}P_{ac})$$

and by the exchange rule (52), this equals

$$(8n)^{-2}\sum_{a,b=1}^{2n}e^{(a+b-c-d)r\pi i/n}\times(1-(-)^{D(a-b)})(1-(-)^{D(c-d)})P_{ac}P_{bd}.$$

The only products which contribute to this sum

are those for which $a\equiv b$ as well as $c\equiv d$, whereby according to (46) and (47)

$$P_{ac}^2=P_{ac}P_{a+n,c+n}=1;\quad P_{ac}P_{a,c+n}=P_{ac}P_{a+n,c}=-C$$

and we obtain

$$(X_r+iY_r)^2=(8n)^{-2}\sum_{a,c=1}^{2n}8e^{2(a-c)r\pi i/n}(1-(-)^rC),$$

whence, observing (62a)

$$X_0^2=\tfrac{1}{2}(1-C)=R_0,$$

$$X_n^2=\tfrac{1}{2}(1-(-)^nC)=R_n=\begin{cases}R_0; & (n\text{ even})\\ 1-R_0; & (n\text{ odd})\end{cases} \tag{66}$$

$$(X_r\pm iY_r)^2=0;\quad (r=1,2,\cdots,n-1). \tag{67}$$

The latter result implies that X_r, Y_r anticommute

$$X_rY_r=-Y_rX_r \tag{67a}$$

and that their squares are identical

$$X_r^2=Y_r^2=R_r. \tag{67b}$$

Now (65b) implies

$$X_rY_r=-Y_rX_r=-iZ_r$$

and since the product in turn must anticommute with either factor, e.g.,

$$X(YX)=(XY)X=-(YX)X,$$

we have similarly

$$Y_rZ_r=-Z_rY_r=-iX_r;\qquad Z_rX_r=-X_rZ_r=-iY_r.$$

These results together imply (67b) as well as its extension

$$Z_r^2=iX_rY_rZ_r=X_r^2=Y_r^2=R_r.$$

The operator R_r thus defined satisfies the relations appropriate to the unit of a quaternion algebra with the hermitian basis (R_r, X_r, Y_r, Z_r), *viz.*, the real basis (R_r, X_r, Y_r, iZ_r) because

$$R_rX_r=Y_rY_rX_r=iY_rZ_r=X_r,$$

etc., and

$$R_r^2=R_rX_rX_r=X_r^2=R_r.$$

The multiplication table is accordingly

$$\begin{aligned}&R_r=R_r^2=X_r^2=Y_r^2=Z_r^2,\\ &X_r=R_rX_r=X_rR_r=iY_rZ_r=-iZ_rY_r,\\ &Y_r=R_rY_r=Y_rR_r=iZ_rX_r=-iX_rZ_r,\\ &Z_r=R_rZ_r=Z_rR_r=iX_rY_r=-iY_rX_r.\end{aligned} \tag{68}$$

For $r=0$ and $r=n$ the operators Y_r and Z_r vanish; in either case we obtain a commutative algebra with a degenerate basis (R_0, X_0) or (R_n, X_n); cf. (66).

In the original quaternion algebra described by (31) the operators R_0, R_1, $\cdots$, R_{n-1}, R_n are projections. It remains to enumerate the dimensions of these projections [in the irreducible representation (30)]. By (66), R_0 and R_n are 2^{n-1} dimensional. By (64), the others have at most that many dimensions, because R_r is contained in R_0 or in $(1-R_0)$ as r is even or odd. Further information can be obtained from suitable explicit expansions of R_r in terms of the basis elements P_{ab}. A very compact expression is obtained by evaluating

$$R_r=\tfrac{1}{2}(X_r^2+Y_r^2)$$

directly from the expansions (62), which yields

$$R_r=2^{-5}n^{-2}\sum_{a,b,c,d=1}^{2n}\cos[(a-b-c+d)r\pi/n]P_{ac}P_{bd}. \tag{69}$$

To obtain an interesting modification of this formula we interchange the pairs of indices (a, b) and (c, d) independently. By (52) the mean of the four alternatives equals

$$\begin{aligned}R_r=2^{-7}n^{-2}\sum_{a,b,c,d}&(\cos((a-b-c+d)r\pi/n)\\ &-(-)^{D(a-b)}\cos((a-b+c-d)r\pi/n))\\ &\times(1+(-)^{D(a-b)+D(c-d)})P_{ac}P_{bd}.\end{aligned}$$

The anticommuting product terms in which either $a\equiv b$ but not $c\equiv d$, or vice versa, cancel out. The terms for which neither congruence is satisfied yield

$$2^{-5}n^{-2}\sum_{a,b,c,d}\sin((a-b)r\pi/n)\sin((c-d)r\pi/n)P_{ac}P_{bd}.$$

The terms for which both congruences are satisfied yield either the identity or $-(-)^rC$ and add up to $\frac{1}{4}(1-(-)^rC)$. Accordingly,

$$\begin{aligned}R_r=(1-(-)^rC)&\\ \times(\tfrac{1}{4}+(8n)^{-2}&\sum_{a,b,c,d=1}^{2n}\sin((a-b)r\pi/n)\\ &\times\sin((c-d)r\pi/n)P_{ac}P_{bd}).\end{aligned} \tag{70}$$

The dimensions (character) of the projection R_r are simply enumerated from (70). When $n>2$,

we have $-1 \neq P_{ac}P_{bd} \neq 1$ unless $a \equiv b$; $c \equiv d$, so that the dimension of R_r is one fourth of the total 2^n.

$$\mathrm{Dim}(R_r) = 2^{n-2}; \quad (r = 1, 2, \cdots, n-1); \quad (n > 2). \quad (71)$$

For the case $n = 2$; $r = 1$ we have from (63c) and (64)

$$B(1+C) = -4X_1; \quad (n = 2).$$

By (43a), the even eigenvectors of B are the two possible even homogeneous functions: (1) and $(\mu_1\mu_2)$; the corresponding characteristic numbers of B are 2 and -2. Neither vanishes, so that in this case R_1 contains all of $1-R_0$, and we have the "exceptional" result

$$R_1 = 1 - R_0; \quad \mathrm{Dim}(R_1) = 2; \quad (n = 2). \quad (71a)$$

Irreducible Representations

In the previous section we have completed the abstract theory of the algebra generated by the operators A and B defined by (27) and (23), which are involved in the eigenwert problem (29). Apart from illustrative references to the representation (30), our main results have been derived from the abstract commutation rules (31). Now the task before us is to apply these results to the solution of problems such as (29), which can be formulated explicitly in terms of A and B. For this purpose we shall again think of the abstract numbers $s_1, s_2, \cdots, s_n, C_1, C_2, \cdots, C_n$ as linear operators in a 2^n-dimensional vector space, defined by the matrix representation (30).

Essentially, the problem of reduction consists in finding the vector spaces which are invariant towards A and B, in the sense that neither A nor B operating on any member of an invariant set can yield anything but a linear combination of the vectors which belong to the same set. Since the set of operators (62) can be constructed from A and B and vice versa [cf. (63c)], it is evident that the invariant sets in question must be invariant towards all the operators (62). In view of the commutation rules (65), we may specify for added convenience that the matrices representing the operators (62) and their products shall be direct products of irreducible representations of the factor groups (R_r, X_r, Y_r, Z_r).

To answer the main questions dealt with in the present communication it will suffice to find the largest solution to the problem (29). The identification of the corresponding irreducible representation of the operators (62) is an easier task than the complete reduction, which we shall leave aside for future attention. We shall go a little further and identify separately for the vector spaces of even and odd functions the representations of maximal dimensions.

By (64) we may consider the sets of even and odd functions separately. The former are annihihilated by (R_r, X_r, Y_r, Z_r) for even $r = (0, 2, 4, \cdots)$, the latter for odd $r = (1, 3, 5, \cdots)$. By (66), the space of even functions is formed by the projection $1 - R_0 = \frac{1}{2}(1+C)$, that of odd functions by $R_0 = \frac{1}{2}(1-C)$.

In the representation (30) the operator of (29) has a matrix whose elements are all positive. Accordingly, by Frobenius' theorem[11] the components of the "maximal" eigenvector must be all of one sign in this representation. It follows immediately that the vector in question cannot be odd. More precisely, it cannot be orthogonal to the even vector

$$\chi_0(\mu_1, \cdots, \mu_n) = \mathrm{const} = 2^{-n/2}$$

(normalized), which happens to be the only function of degree zero. By (43a), this is an eigenvector of B corresponding to the simple characteristic number n

$$(B, \chi_0) = (B(1-R_0), \chi_0) = n\chi_0. \quad (72)$$

Since by (63c) and (64)

$$\begin{aligned} -B &= X_1 + X_2 + \cdots + X_{2n}, \\ -B(1-R_0) &= X_1 + X_3 + \cdots + X_{2n-1} \\ &= \begin{cases} 2X_1 + 2X_3 + \cdots + 2X_{2m-1}; \\ \qquad\qquad (n = 2m) \\ 2X_1 + 2X_3 + \cdots + 2X_{2m-1} \\ \quad + X_{2m+1}; \quad (n = 2m+1) \end{cases} \end{aligned} \quad (73)$$

and $X_0, X_1, \cdots, X_n$ commute with each other, they commute with B. Accordingly, operation with X_r on χ_0 will either annihilate it or convert it into some function of the same degree. But χ_0 is the only function of degree zero. Hence, χ_0 is a common eigenvector of $X_0, X_1, \cdots X_n$ satisfying

$$(X_r, \chi_0) = \xi_r\chi_0; \quad (r = 0, 1, \cdots, n).$$

By (68) and (66) the operators X_r all satisfy the identity

$$X_r^3 - X_r = X_r(X_r-1)(X_r+1) = 0, \qquad (74)$$

so that $\xi_0, \xi_1, \cdots, \xi_n$ are to be selected from the numbers 0, 1, -1. Since χ_0 is an even vector we have

$$\xi_0 = \xi_2 = \xi_4 = \cdots = 0$$

and by comparison with (73)

$$\xi_1 + \xi_3 + \cdots + \xi_{2n-1} = -n.$$

There is just one way to satisfy this requirement

$$\begin{gathered} \xi_1 = \xi_3 = \cdots = \xi_{2n-1} = -1, \\ (X_r, \chi_0) = -\chi_0; \\ (r = 1, 3, \cdots, 2[(n-1)/2]+1). \end{gathered} \qquad (75)$$

Having identified one common eigenvector χ_0 of $X_1, X_3, \cdots$, we proceed to construct others which belong to the same invariant set by operations with $Y_1, Y_3, \cdots$. In general if χ satisfies

$$(X_r, \chi) = \xi_r \chi; \quad (r = 1, 3, \cdots),$$

then by (68) and (65)

$$\begin{aligned} (X_r, (Y_r, \chi)) &= (X_r Y_r, \chi) = (-Y_r X_r, \chi) \\ &= -\xi_r (Y_r, \chi), \\ (X_s, (Y_r, \chi)) &= (X_s Y_r, \chi) = (Y_r X_s, \chi) \\ &= \xi_s (Y_r, \chi); \quad (s \neq r) \end{aligned}$$

so that the operation with Y_r gives a new common eigenvector; the sign of the corresponding ξ_r is reversed and the others are unchanged. If ξ_r vanishes, Y_r will only annihilate χ because by (68)

$$(Y_r, \chi) = (Y_r X_r^2, \chi) = (Y_r, \xi_r^2 \chi).$$

For this reason it is useless to operate with $Y_2, Y_4, \cdots$ on χ_0. It is equally useless to operate more than once with any one Y_r because by (68) Y_r is its own inverse in the subspace R_r

$$Y_r^2 = X_r^2 = R_r,$$

so that the second operation at best undoes the effect of the first. Finally, since

$$Z_r = iX_r Y_r$$

the operation with Z_r can only give us such eigenfunctions of X_r as we can obtain with Y_r alone. Accordingly, the vectors which we can obtain by operating with various combinations of $(Y_1, Y_3, \cdots)$ on χ_0—at most once apiece—form an invariant set. The vectors thus obtained can be distinguished from each other by their different sets of characteristic numbers; when necessary we shall designate them individually

$$\chi(\xi_1, \xi_3, \cdots, \xi_{2m-1}; (\mu)); \quad (n \geqq 2m \geqq n-1).$$

In the case of odd n we have $\xi_n = -1$ for every vector in the set; there is no Y_n. For the rest, every combination occurs exactly once, as is expressed by the following formulation of the relations derived above

$$\begin{aligned} &(X_r, \chi(\xi_1, \xi_3, \cdots, \xi_{2m-1}; (\mu))) \\ &\qquad = \xi_r \chi(\xi_1, \xi_3, \cdots, \xi_{2m-1}; (\mu)), \\ &(Y_r, \chi(\xi_1, \xi_3, \cdots, \xi_{2m-1}; (\mu))) \\ &\qquad = \chi(\xi_1, \cdots, -\xi_r, \cdots, \xi_{2m-1}; (\mu)), \\ &(X_n, \chi(\xi_1, \xi_3, \cdots, \xi_{n-2}; (\mu))) \\ &\qquad = -\chi(\xi_1, \cdots, \xi_{n-2}; (\mu)). \end{aligned} \qquad (76)$$

A more explicit description of the functions χ is not necessary. The relations (76) in conjunction with the verified construction of the one vector

$$\chi(-1, -1, \cdots, -1; (\mu)) = 2^{-n/2} \qquad (76a)$$

suffice for definition. From the one given vector, the construction is in effect completed by means of the formal relations (68).

The representation (76) is analogous to (30); but it has only $m = [n/2]$ factors and the number of dimensions is $2^{[n/2]}$, if we denote by $[x]$ the greatest integer which does not exceed x. Moreover, denoting by Q_r a general function of the factor basis (R_r, X_r, Y_r, Z_r), the representation (76) is a direct product of the two-dimensional representations

$$\begin{aligned} &\mathbf{D}_{\max} = \mathbf{D}_2(Q_1) \times \mathbf{D}_2(Q_3) \times \cdots \times \mathbf{D}_2(Q_{n-1}); \\ &\qquad\qquad (n = 2m) \\ &\mathbf{D}_{\max} = \mathbf{D}_2(Q_1) \times \mathbf{D}_2(Q_3) \times \cdots \\ &\qquad \times \mathbf{D}_2(Q_{n-2}) \times \mathbf{D}_-(Q_n); \quad (n = 2m+1) \\ &\mathbf{D}_2(X_r) = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}; \quad \mathbf{D}_2(Y_r) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \\ &\mathbf{D}_+(X_r) = (1); \quad \mathbf{D}_-(X_r) = (-1) \end{aligned} \qquad (77)$$

supplemented by the one-dimensional representation $\mathbf{D}_-(Q_n)$ when n is odd.

An invariant vector space may be constructed by the same procedure from any common eigenvector of $(X_0, X_1, \cdots, X_n)$. The characters of the representation will be determined by the initial ξ_0 and ξ_n, which are common to all members of an invariant set, together with the values (0 or 1) of $\xi_1^2, \xi_2^2, \cdots, \xi_{n-1}^2$. For the signs of $\xi_1, \xi_2, \cdots, \xi_{n-1}$ can be changed independently by operation with $Y_1, Y_2, \cdots, Y_{n-1}$, excepting those which vanish in the first place. To put it in geometrical language, the general type of the representation is determined by an intersection of projections

$$P_0P_1\cdots P_n$$

where for $r=1, 2, \cdots, n-1$, P_r is either R_r or $1-R_r$, while R_0 is subdivided into $\frac{1}{2}(R_0+X_0)$ and $\frac{1}{2}(R_0-X_0)$, and R_n is similarly subdivided. The vector space constructed above from χ_0 is the only intersection common to all of the projections $R_1, R_3, \cdots, R_{[n/2]-1}$. For every such intersection must contain an even eigenvector of B corresponding to the characteristic number n when n is even or $n-1-\xi_n$ when n is odd, in either case an even function of degree less than 2, and the only function that satisfies this specification is const. $=\chi_0$.

We have already pointed out that by Frobenius' theorem, that eigenvector which corresponds to the largest solution of (29) cannot be orthogonal to χ_0. Therefore, this eigenvector belongs to the invariant set constructed above, which contains χ_0. The expectation of a *simple* largest characteristic number is in accord with our finding that the invariant vector space which corresponds to the maximal representation (77) is unique.

In connection with the considerations of Lassettre and Howe,[13] it ia a matter of interest to identify not only the largest solution $\lambda_{\max}$ of (29), but in addition the largest solution $\bar{\lambda}_{\max}$ which belongs to an *odd* eigenvector. As it happens, this solution is the second largest in magnitude. We shall prefer a slight variation of the above procedure. From one common eigenvector of the operators

$$X_r^* = -X_r\cos(r\pi/n) + Y_r\sin(r\pi/n); \quad (r=0, 1, \cdots, n-1, n) \tag{78}$$
$$X_0^* = -X_0; \quad X_n^* = X_n$$

we shall construct others by operations with, say, $Z_1, \cdots, Z_{n-1}$, which anticommute with the corresponding X_r^*. Then instead of B we consider

$$A = \sum_{j=1}^{n} s_j s_{j+1} = -\sum_{r=1}^{2n} X_r^* = X_0 - \sum_{r=1}^{n-1} 2X_r^* - X_n,$$
$$R_0 A = \tfrac{1}{2}(1-C)A \tag{79}$$
$$= \begin{cases} X_0 - 2X_2^* - 2X_4^* - \cdots - 2X_{n-2}^* - X_n; & (n=2m) \\ X_0 - 2X_2^* - 2X_4^* - \cdots - 2X_{n-1}^*; & (n=2m+1) \end{cases}$$

[cf. (63c)]. By (68) the operators (78) satisfy

$$X_r^{*2} = R_r = X_r^2; \quad X_r^{*3} - X_r^* = 0. \tag{80}$$

The matrix which represents the operator

$$\exp(H'A) = \prod_{j=1}^{n} (\cosh H' + s_j s_{j+1} \sinh H')$$

in terms of the vector basis (41) which renders B diagonal consists of two 2^{n-1}-dimensional matrices which transform even functions among themselves and odd functions among themselves, respectively. In either matrix all elements are positive (provided $H'>0$), so that Frobenius' theorem applies in the vector spaces of even and odd functions separately. The modification by the factor $\exp(H^*B)$ in (29) does not affect this conclusion because this factor is represented here by a diagonal matrix whose elements are all positive.

By (44) the largest characteristic number n of A is double and belongs to the two configurations $(+, +, \cdots, +)$, $(-, -, \cdots, -)$, which are free from alternations of sign. When the corresponding even and odd eigenvectors

$$\left.\begin{matrix} \chi_0^* \\ \chi_0^{(-)*} \end{matrix}\right\} = 2^{-\frac{1}{2}}(2^{-n}\prod_{1}^{n}(1+\mu_j) \pm 2^{-n}\prod_{1}^{n}(1-\mu_j)) \tag{81}$$

are expanded in terms of the vector basis (41), their components are all positive, so that the representations which correspond to the characteristic numbers $\lambda_{\max}$ and $\bar{\lambda}_{\max}$ of (29) must

[13] E. N. Lassettre and J. P. Howe, reference 12.

belong to unique invariant vector spaces which contain $\chi_0{}^*$ and $\chi_0{}^{(-)*}$, respectively. The former has been constructed above from χ_0. The odd vector $\chi_0{}^{(-)*}$ is a common eigenvector of all $X_r{}^*$ and satisfies

$$n\chi_0{}^{(-)*}=(A,\ \chi_0{}^{(-)*})$$
$$=-\sum_{q=1}^{n}(X_{2q}^*,\ \chi_0{}^{(-)*})=-\left(\sum_{q=1}^{n}\xi_{2q}^*\right)\chi_0{}^{(-)*}$$

which requires

$$\xi_0=-\xi_0{}^*=1,$$
$$\xi_{2q}^{*2}=1;\quad (0<q<\tfrac{1}{2}n)$$
$$\xi_n=\xi_n{}^*=-1;\quad (n=2m),$$

so that the vector $\chi_0{}^{(-)*}$ is included in the projection

$$\tfrac{1}{2}(R_0+X_0)R_2R_4\cdots R_{2[n/2]}$$

and in $\frac{1}{2}(R_n-X_n)$ when n is even. The "maximal odd" representation is therefore

$$\mathbf{D}_{\max}^{-}=\mathbf{D}_+(Q_0)\times\mathbf{D}_2(Q_2)\times\cdots\times\mathbf{D}_2(Q_{n-1});\quad (n=2m+1)$$
$$\mathbf{D}_{\max}^{-}=\mathbf{D}_+(Q_0)\times\mathbf{D}_2(Q_2)\times\cdots\times\mathbf{D}_2(Q_{n-2})\times\mathbf{D}_-(Q_n);\quad (n=2m) \tag{82}$$

with the notation of (77). When n is odd, $\mathbf{D}_{\max}^{-}$ has $2^{(n-1)/2}$ dimensions, the same number as $\mathbf{D}_{\max}$, and there can be no further representation with this number of dimensions, for there is only one pair of configurations with less than two alternations of sign. For even n the representation $\mathbf{D}_{\max}^{-}$ has only $2^{(n-2)/2}$ dimensions; it is still unique. However, one other representation with the same number of dimensions is compatible with the known spectrum (44) of A, namely,

$$\mathbf{D}_{\text{alt}}=\mathbf{D}_-(Q_0)\times\mathbf{D}_2(Q_2)\times\cdots\times\mathbf{D}_2(Q_{n-2})\times\mathbf{D}_+(Q_n). \tag{82a}$$

The count of configurations with n (even) alternations yields one pair: $(+\ -\ +\ -\ \cdots\ +\ -)$ and $(-\ +\ -\ +\ \cdots\ -\ +)$; reasoning analogous to the above shows that exactly one invariant vector space belongs to (82a).

The identification of the remaining invariant vector spaces involves more elaborate calculations; the complete theory will be given in a later publication. However, in order to settle an interesting question which will arise, we shall complete the discussion of those n vector spaces which contain the n functions of degree one

$$\chi_1(2r;\ \mu_1,\ \cdots,\ \mu_n)=n^{-\frac{1}{2}}\sum_{k=1}^{n}\exp(2rk\pi i/n)\mu_k. \tag{83a}$$

These functions may be classified according to the representations of the dihedral symmetry group (55). To the identical representation of (55) belongs $\chi_1(0;\ (\mu))$; the corresponding representation of the algebra (68) is (82). For even n, $\chi_1(n;\ (\mu))$ belongs to another one-dimensional representation of (55) and to the representation (82a) of (68). The remaining functions (83a) belong pairwise to two-dimensional representations of (55). To show that the pair of similar representations which belong to the pair $\chi_1(\pm 2r;\ (\mu))$ are described by

$$\mathbf{D}_-(Q_0)\times\mathbf{D}_0(Q_{2r})\times\prod_{s\neq r}\mathbf{D}_2(Q_{2s});\quad (n\text{ odd})$$
$$\mathbf{D}_-(Q_0)\times\mathbf{D}_-(Q_n)\times\mathbf{D}_0(Q_{2r})\times\prod_{s\neq r}\mathbf{D}_2(Q_{2s});\quad (n\text{ even}) \tag{83b}$$

one may verify that the vectors in question are annihilated by X_{2r}

$$(X_{2r},\ \chi_1(2r;\ (\mu)))=(X_{2r},\ \chi_1(-2r;\ (\mu)))=0;\quad (0<2r<n). \tag{83c}$$

The direct calculation by means of (62) and (54) is not too laborious; since X_{2r} commutes with B, only the terms of first degree have to be computed. The remaining factors in (83b) are then determined as before by the relation

$$(B,\ \chi_1)=(n-2)\chi_1.$$

SOLUTION OF THE EIGENWERT PROBLEM

It is a simple matter now to compute those solutions of the eigenwert problem (29) which belong to the representations (77), (82), and (83); we only have to solve a set of quadratic equations.

As to the "physical" significance of the solutions, we recall that the characteristic number itself yields the partition function and with it the thermodynamic functions of the crystal. Moreover, as shown by Kramers and Wannier, the individual components $\psi(\mu_1,\ \cdots,\ \mu_n)$ of the

eigenvector which belongs to $\lambda_{\max}$ describe the statistical distribution of configurations of the last tier of atoms added to the crystal.[10] On the other hand, if we know in addition the eigenvector $\psi'(\mu_1, \cdots, \mu_n)$ which belongs to $\lambda_{\max}$ for the adjoint operator $V' = V_1' V_2' = V_1 V_2$, then the component products

$$\psi(\mu_1, \cdots, \mu_n)\psi'(\mu_1, \cdots, \mu_n)$$

describe the statistical distribution of configurations in the *interior* of the crystal.[13]

With the latter result in mind, we first transform V to self-adjoint form by operation with $V_1^{\frac{1}{2}}$; then

$$\bar{V} = V_1^{\frac{1}{2}} V V_1^{-\frac{1}{2}} = V_1^{\frac{1}{2}} V_2 V_1^{\frac{1}{2}}$$
$$= (2 \sinh 2H)^{n/2} \times \exp(\tfrac{1}{2}H'A) \exp(H^*B) \exp(\tfrac{1}{2}H'A) \quad (84)$$

has the same characteristic numbers as V, and the squares

$$\psi^2(\mu_1, \cdots, \mu_n) = f(\mu_1, \cdots, \mu_n)$$

of the components of its principal eigenvector will describe the distribution of configurations in the interior of the crystal.

To solve the eigenwert problem we may transform $\bar{V}$ into a function of the operators $X_0, X_1, \cdots, X_n$ alone, or equally well into a function of $X_0^*, X_1^*, \cdots, X_n^*$. The latter procedure involves slightly simpler relations; either result is readily converted into the other by means of the real orthogonal operator[14]

$$\exp\left(\sum_{r=1}^{n-1} ((n-r)/2n)\pi i Z_r\right)$$
$$= \prod_{r=1}^{n=1} (1-(1-\sin(r\pi/2n))R_r + \cos(r\pi/2n) i Z_r).$$

For reference we observe here the somewhat more general rule

$$\exp(i\alpha Z_r)(X_r \cos\beta + Y_r \sin\beta) \exp(-i\alpha Z_r)$$
$$= X_r \cos(2\alpha+\beta) + Y_r \sin(2\alpha+\beta) \quad (85)$$

which is easily verified by means of the multiplication table (68). The latter—and (85)—are also valid if X_r, Y_r, Z_r are replaced throughout by

$$X_r^* = -X_r \cos(r\pi/n) + Y_r \sin(r\pi/n),$$
$$Y_r^* = X_r \sin(r\pi/n) + Y_r \cos(r\pi/n), \quad (86)$$
$$Z_r^* = -Z_r$$

(dual transformation). We now recall the expansions

$$A = -X_0^* - 2X_1^* - \cdots - 2X_{n-1}^* - X_n^*$$
$$B = -X_0 - 2X_1 - \cdots - 2X_{n-1} - X_n$$
$$= X_0^* + 2\sum_{r=1}^{n-1} (\cos(r\pi/n) X_r^* - \sin(r\pi/n) Y_r^*) - X_n^*.$$

Substitution in (84) yields

$$\bar{V} = (2 \sinh 2H)^{n/2} \exp((H^*-H')X_0^*) \prod_{r=1}^{n-1} (U_r) \exp(-(H^*+H')X_n^*) \quad (87)$$

where

$$U_r = \exp(-H'X_r^*) \exp(-2H^*X_r) \exp(-H'X_r^*)$$
$$= (1-R_r) + (\cosh 2H' \cosh 2H^* - \sinh 2H' \sinh 2H^* \cos(r\pi/n))R_r$$
$$- (\sinh 2H' \cosh 2H^* - \cosh 2H' \sinh 2H^* \cos(r\pi/n))X_r^*$$
$$- \sinh 2H^* \sin(r\pi/n) Y_r^*. \quad (87a)$$

By inspection of the factored form we note that transformation with $(1-R_r+iZ_r)$ changes U_r into U_r^{-1}, which differs from U_r in the signs of the coefficients of X_r^* and Y_r^*. Adding the two together we obtain

$$U_r + U_r^{-1} = 2(1-R_r + (\cosh 2H' \cosh 2H^* - \sinh 2H' \sinh 2H^* \cos(r\pi/n))R_r)$$
$$= 2(1-R_r) + 2 \cosh \gamma_r R_r$$

whence the characteristic numbers of U_r belonging to the subspace R_r are e^{γ_r} and $e^{-\gamma_r}$, of equal multiplicity. (Those which belong to $(1-R_r)$ are trivial, all equal to unity.) Accordingly we may write

$$U_r = 1 - R_r + \cosh\gamma_r R_r - \sinh\gamma_r \cos\delta_r^* X_r^* - \sinh\gamma_r \sin\delta_r^* Y_r^*$$
$$= \exp(-\gamma_r(\cos\delta_r^* X_r^* + \sin\delta_r^* Y_r^*)) \quad (88)$$

where γ_r and δ_r^* can be computed from $2H'$,

[14] This is not exactly the dual transformation; it takes a further transformation with $\Pi(1-R_r+X_r)$ to obtain (86).

$2H^*$, $\omega_r = r\pi/n$ by the rules of hyperbolic trigonometry, as indicated by Fig. 4. We note in particular the trigonometric relations[15]

$$\begin{aligned}
\cosh\gamma &= \cosh 2H' \cosh 2H^* \\
&\quad - \sinh 2H' \sinh 2H^* \cos\omega, \quad \text{(a)} \\
\sinh\gamma \cos\delta^* &= \sinh 2H' \cosh 2H^* \\
&\quad - \cosh 2H' \sinh 2H^* \cos\omega, \quad \text{(b)} \\
\sin\omega/\sinh\gamma &= \sin\delta^*/\sinh 2H^* \\
&= \sin\delta'/\sinh 2H', \quad \text{(c)} \\
\cot\delta^* &= (\sinh 2H' \coth 2H^* \\
&\quad - \cosh 2H' \cos\omega)/\sin\omega. \quad \text{(d)}
\end{aligned} \tag{89}$$

With the aid of (85) and (86) we find immediately the transformations which reduce U_r to diagonal form with regard to the eigenvectors of either X_r^* or X_r as a vector basis,

$$U_r = \exp(-\tfrac{1}{2}\delta_r^* i Z_r)\exp(-\gamma_r X_r^*)\exp(\tfrac{1}{2}\delta_r^* i Z_r), \tag{90a}$$

$$\begin{aligned}
U_r &= \exp(\tfrac{1}{2}(\pi-\omega_r \\
&\quad -\delta_r^*) i Z_r)\exp(-\gamma_r X_r)\exp(-\tfrac{1}{2}(\pi-\omega_r-\delta_r^*) i Z_r), \\
&\qquad (r=1, 2, \cdots, n-1)
\end{aligned} \tag{90b}$$

and by substitution in (87)

$$\begin{aligned}
&\exp\left(\sum_{r=1}^{n-1}\tfrac{1}{2}\delta_r^* i Z_r\right)\bar{V}\exp\left(-\sum_{r=1}^{n-1}\tfrac{1}{2}\delta_r^* i Z_r\right) \\
&= (2\sinh 2H)^{n/2}\exp\Big((H^*-H')X_0^* \\
&\qquad -\sum_{r=1}^{n-1}\gamma_r X_r^* - (H'+H^*)X_n^*\Big),
\end{aligned} \tag{91a}$$

$$\begin{aligned}
&\exp\Big(-\sum_{r=1}^{n-1}\tfrac{1}{2}(\pi-\omega_r \\
&\qquad -\delta_r^*) i Z_r\Big)\bar{V}\exp\Big(\sum_{r=1}^{n-1}\tfrac{1}{2}(\pi-\omega_r-\delta_r^*) i Z_r\Big) \\
&= (2\sinh 2H)^{n/2}\exp\Big((H'-H^*)X_0 \\
&\qquad -\sum_{r=1}^{n-1}\gamma_r X_r - (H'+H^*)X_n\Big).
\end{aligned} \tag{91b}$$

[15] The formulas of hyperbolic trigonometry are obtained from those of spherical trigonometry by the substitution of imaginary lengths for the sides. See F. Klein, *Vorlesungen über Nicht-Euklidische Geometrie* (Springer, Berlin, 1928), p. 195.

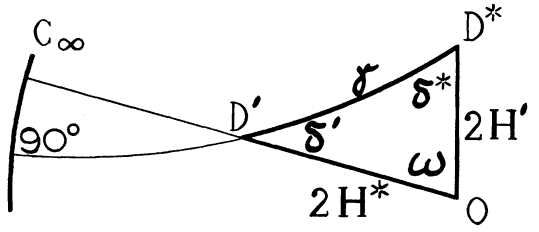


FIG. 4. Hyperbolic triangle. Stereographic projection, conformal. Circles are represented by circles, geodetics by circles invariant towards inversion in the limiting circle $C\infty$ of the projection. See F. Klein, reference 15, pp. 293–299.

The spectrum of $\bar{V}$ is now known to the extent that the common eigenvectors χ of $(X_0, X_1, \cdots, X_{n-1}, X_n)$ and the corresponding sets of characteristic numbers $(\xi_0, \xi_1, \cdots, \xi_{n-1}, \xi_n)$ are known. For every solution χ to that problem $\bar{V}$ has an eigenvector ψ with characteristic number λ given by

$$\begin{aligned}
\psi &= \left(\exp\left(-\sum_{r=1}^{n-1}\tfrac{1}{2}(\pi-\omega_r-\delta_r^*) i Z_r\right), \chi\right), \\
(\bar{V}, \psi) &= \lambda\psi, \\
\log\lambda &= \tfrac{1}{2}n\log(2\sinh 2H) + (H'-H^*)\xi_0 \\
&\quad -\sum_{r=1}^{n-1}\gamma_r\xi_r - (H'+H^*)\xi_n.
\end{aligned} \tag{92}$$

In the previous section we were able to show that the largest characteristic number of $\bar{V}$ belongs to the representation (77). In view of (76) and (76a) we must put $\xi_0=\xi_2=\xi_4=\cdots=0$. All the others may be taken negative, which calls for $\chi=\chi_0$, and obviously this is the best choice. Accordingly,

$$\begin{aligned}
&\log\lambda_{\max} - \tfrac{1}{2}n\log(2\sinh 2H) \\
&= \begin{cases} \gamma_1+\gamma_3+\cdots+\gamma_{2m-1}; & (n=2m) \\ \gamma_1+\gamma_3+\cdots+\gamma_{2m-1}+(H'+H^*); & (n=2m+1). \end{cases}
\end{aligned} \tag{93}$$

These two results can be combined if we adopt the natural conventions

$$\gamma_{-r} = \gamma_r; \quad \gamma_n = 2H'+2H^*. \tag{94}$$

Then (93) takes the compact form

$$\begin{aligned}
&\log\lambda_{\max} - \tfrac{1}{2}n\log(2\sinh 2H) = \tfrac{1}{2}\sum_{r=1}^{n}\gamma_{2r-1} \\
&= \tfrac{1}{2}\sum_{r=1}^{n}\cosh^{-1}(\cosh 2H'\cosh 2H^* \\
&\quad -\sinh 2H'\sinh 2H^*\cos((2r-1)\pi/2n)).
\end{aligned} \tag{95}$$

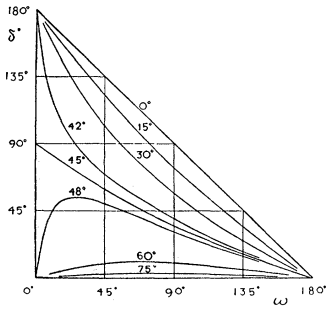


FIG. 5. Variation of δ^* with ω for the quadratic crystal, at various reduced temperatures $(k/J)T=1/H$.

gd $2H$	$1/H$
0°	∞
15°	7.551
30°	3.641
42°	2.472
45°	2.269
48°	2.089
66°†	1.29
77°‡	0.92

† By mistake marked 60° on figure.
‡ By mistake marked 75° on figure.

The corresponding eigenvector can be described by either of the two formulas

$$\psi_{\max}=\left(\exp\left(-\sum_{0<2r<n}\tfrac{1}{2}(\pi-\omega_{2r-1}-\delta^*_{2r-1})iZ_{2r-1}\right),\chi_0\right), \quad (96a)$$

$$\psi_{\max}=\left(\exp\left(\sum_{0<2r<n}\tfrac{1}{2}\delta^*_{2r-1}iZ_{2r-1}\right),\chi_0^*\right). \quad (96b)$$

Here we have omitted operations with $\exp((\text{const})Z_{2r})$; $(r=1, 2, \cdots)$, because these have no effect on χ_0 or any other even vector. The somewhat simpler form (96b) involves construction from the even δ function χ_0^* given by (81); one easily verifies that ξ_1^*, ξ_3^*, $\cdots$ are all negative for this vector.

The Principal Eigenvector

The result (96) describes explicitly the distribution of configurations (ψ^2) of one row of atoms in a crystal. The terms of the description are quite unfamiliar. We should not regret this; for among the main objects of the development of this theory is the invention of more suitable methods for the description of such distributions. Even so, we must try to establish the connection with more familiar types of description in terms of more tangible quantities. Moreover, the result (96) fails to describe the statistical correlation of configurations in different rows of atoms. Methods of dealing with these two tasks have been perfected to a considerable degree; but the algebraic apparatus involved is elaborate enough to make a separate publication advisable.

One quite tangible result is readily obtained from (96b): The probability of a configuration free from alternations is

$$2\psi^2(++\cdots+)=2\psi^2(--\cdots-)=\prod(\cos^2(\tfrac{1}{2}\delta^*_{2r-1})).$$

Similarly, when n is even so that a configuration free from persistencies of sign is possible, the probability of such a configuration is

$$2\psi^2(+-+-\cdots+-)=2\psi^2(-+-+\cdots-+)=\prod(\sin^2(\tfrac{1}{2}\delta^*_{2r-1})).$$

Presumably, the probabilities of the 2^n-4 remaining configurations are intermediate between the given limits. One can show from the commutation rules that the probabilities of configurations with 2, 4, 6, $\cdots$ alternations of sign can be computed successively from those terms in the expansion of (96b) which contain, respectively, 1, 2, 3, $\cdots$ factors of the type $(Z_r \sin\tfrac{1}{2}\delta_r^*)$. However, the labor involved increases rapidly with the number of steps.

Of greater interest is the fact that the description (96) brings out a striking qualitative difference between those distributions which occur for $n(H'-H^*)\gg 1$ and those which occur for $n(H^*-H')\gg 1$.

The variation of δ^* with $\omega=r\pi/n$ is given analytically by (89d); but a qualitative inspection of Fig. 4 is even more convenient. Let us keep the side $OD^*=2H'$ of the triangle OD^*D' fixed; then the positions of the vertex D' for $\omega=\pi/n$, $\omega=3\pi/n$, $\cdots$ are equidistant points on a circle of radius $OD'=2H^*$. Now if $2H^*>2H'$, then $\delta^*=\pi$ for $\omega=0$, and δ^* decreases from π to 0 as ω increases from 0 to π. On the other hand, if $2H^*<2H'$, then $\delta^*=0$ for $\omega=0$. As ω increases, δ^* increases to a maximum value

$$\sin^{-1}(\sinh 2H^*/\sinh 2H')=\delta^*_{\max}<\tfrac{1}{2}\pi$$

given by (89c) for $\delta'=\frac{1}{2}\pi$; with further increase of ω, δ^* decreases again until $\delta^*=0$ for $\omega=\pi$.

As regards the angle $\frac{1}{2}(\pi-\delta^*-\omega)$ which occurs in (96a), the axiom

$$\delta'+\delta^*+\omega<\pi$$

of hyperbolic geometry implies

$$\pi-\omega-\delta^*>0.$$

A graphical representation of δ^* as a function of ω at various temperatures is given in Fig. 5 for a quadratic crystal ($H'=H$). As regards the variation of δ^* with the temperature for a fixed ω, we note that as the former increases from 0 to ∞, δ^* increases from 0 to $\pi-\omega$. *For small values of ω, nearly all of this increase takes place over a small interval of temperatures which includes the critical point.* A detailed inspection of the operators Z_r can be made to show that those for which r is small are the most effective in introducing pairs of alternations far apart, which is just what it takes to convert order into disorder.

Concerning the extreme cases of low and high temperatures, one sees easily that in the former case δ^* and in the latter case $\pi-\omega-\delta^*$ will remain small for all ω. This is neither new nor surprising; it means that the low temperature distribution consists mostly of configurations which resemble the perfectly ordered arrangement represented by $\chi_0{}^*$, while the high temperature distribution resembles the completely random distribution described by χ_0.

Propagation of Order

The principal characteristic number (95) of the eigenwert problem (29) yields the partition function, and the principal eigenvector determines the distribution of configurations. Nevertheless, the remaining 2^n-1 characteristic numbers are of some interest. In general, these describe the propagation of order.[16] In particular, if long-range order is present, at least one of the subsidiary characteristic numbers should be very nearly equal to the principal.[17] Moreover, at the transition point where long-range order appears, one may expect a phenomenon analogous to the branching of multiple-valued analytic functions such as $z^{1/n}$, whereby the order of the branch-point bears a relation to the type of the singularity. A survey of the solutions which belong to the representations (77), (82), and (83) will answer the most important questions.

To obtain all the solutions which belong to (77b), the angles $\frac{1}{2}\delta_1{}^*$, $\frac{1}{2}\delta_3{}^*$, $\cdots$ in (96) may be replaced independently by $\frac{1}{2}\delta_1{}^*+\frac{1}{2}\pi$, $\frac{1}{2}\delta_3{}^*+\frac{1}{2}\pi$, $\cdots$; the corresponding characteristic numbers are given by the formula

$$\log\lambda-\tfrac{1}{2}n\log(2\sinh 2H)=\begin{cases}\pm\gamma_1\pm\gamma_3\pm\cdots\pm\gamma_{2m-1}; & (n=2m)\\ \pm\gamma_1\pm\gamma_3\pm\cdots\pm\gamma_{2m-1}+\frac{1}{2}\gamma_{2m+1}; & (n=2m+1)\end{cases}\tag{97}$$

where the optional signs are independent and each combination occurs once.

That part of the spectrum of V which belongs to the representation (82) is obtained similarly. The result is

$$\log\lambda-\tfrac{1}{2}n\log(2\sinh 2H)=\begin{cases}(H'-H^*)\pm\gamma_2\pm\gamma_4\pm\cdots\pm\gamma_{2m-2}+\frac{1}{2}\gamma_{2m}; & (n=2m)\\ (H'-H^*)\pm\gamma_2\pm\gamma_4\pm\cdots\pm\gamma_{2m}; & (n=2m+1).\end{cases}\tag{98}$$

For the largest of these we find the counterpart of (95)

$$\log\lambda_{\max}^{(-)}-\tfrac{1}{2}n\log(2\sinh 2H)=(H'-H^*)+\tfrac{1}{2}\sum_{r=1}^{n-1}\gamma_{2r}=\tfrac{1}{2}\Big(\gamma_0\operatorname{sgn}(H'-H^*)+\sum_{r=1}^{n-1}\gamma_{2r}\Big)\tag{99}$$

with the natural notation

$$\gamma_0=\cosh^{-1}(\cosh 2H'\cosh 2H^*-\sinh 2H'\sinh 2H^*)=2|H'-H^*|.\tag{100}$$

First of all, this differs from (95) in the substitution of γ_0, γ_2, $\cdots$ for γ_1, γ_3, $\cdots$. Moreover, the sign of $\frac{1}{2}\gamma_0$ is mandatory and changes at the critical point. This leads to a most remarkable limiting result for large values of n. The two sums

$$\gamma_1+\gamma_3+\cdots+\gamma_{2n-1}=\gamma(\pi/n)+\gamma(3\pi/n)+\cdots,$$
$$\gamma_0+\gamma_2+\cdots+\gamma_{2n-2}=\gamma(0)+\gamma(2\pi/n)+\cdots$$

[16] F. Zernike, Physica **7**, 565 (1938).

[17] See reference 13. See also E. Montroll, J. Chem. Phys. **10**, 61 (1942).

may be considered as different numerical quadratures of

$$(n/2\pi)\int_0^{2\pi}\gamma(\omega)d\omega$$

by the trapeze rule. For periodic, analytic functions the approximation to the integral improves very rapidly (exponentially) with increasing number of intervals. Hence, with rapid convergence

$$\lim_{n=\infty}(\lambda_{\max}^{(-)}/\lambda_{\max})=\begin{cases}1; & (H'>H^*)\\ \exp(2H^*-2H'); & (H'<H^*).\end{cases} \tag{101}$$

The distribution of the logarithms of the remaining characteristic numbers which belong to (77) and (82)

$$\log\lambda_{\max}-2\gamma_1,\ \log\lambda_{\max}-2\gamma_3,\ \cdots,\ \log\lambda_{\max}-2\gamma_1-2\gamma_3,\ \cdots,$$
$$\log\lambda_{\max}^{(-)}-2\gamma_2,\ \log\lambda_{\max}^{(-)}-2\gamma_4,\ \cdots,\ \log\lambda_{\max}^{(-)}-2\gamma_2-2\gamma_4,\ \cdots$$

becomes *dense* as $n\to\infty$. These "continua" remain distinct from the two largest characteristic numbers as long as $H'\neq H^*$. However, for $H'<H^*$ the representations (83b) give rise to a continuum

$$\log\lambda=\log\lambda_{\max}^{(-)}+\gamma_0-\gamma_{2r};\quad (H'<H^*) \tag{102}$$

which contains $\lambda_{\max}^{(-)}$ as a superior limit. Further complications due to representations which we have not investigated here are excluded by (43) and (63c).

At the critical point $H'=H^*$, we have $\gamma_0=0$; $\gamma_r=O(r/n)$. In this exceptional case both $\lambda_{\max}^{(-)}$ and $\lambda_{\max}$ itself are limits of "continua." The following scheme summarizes the results

$$\begin{aligned}&\lambda_{\max}=\lambda_{\max}^{(-)}>\text{(continuum)};\quad (H'>H^*)\\ &\lambda_{\max}=\lambda_{\max}^{(-)}=\lim\text{ (continuum)};\quad (H'=H^*)\\ &\lambda_{\max}>\lambda_{\max}^{(-)}=\lim\text{ (continuum)};\quad (H'<H^*).\end{aligned} \tag{103}$$

At temperatures below the critical point ($H'>H^*$), we have "asymptotic degeneracy" of order 2, as a symptom of long-range order. Above the critical point, there is no degeneracy of the principal characteristic number. At the critical point we observe branching associated with an "asymptotic degeneracy" of *infinite order*.

In regard to the "propagation of order," the mean distance to which a local disturbance in the crystal is propagated is inversely proportional to $\log(\lambda_{\max}/\lambda)$. We note that this "range" of the "short-range order" becomes infinite at the critical point.

Since the functions (83a) belong to different representations of the dihedral group (55), —and the same is necessarily true for their respective invariant vector spaces—, the result (102) ought to contain information about the anisotropy of the propagation of order. A tentative computation leads to the implicit formula

$$\cosh 2H\cosh 2H'-\sinh 2H\cosh(\beta\sin\varphi)-\sinh 2H'\cosh(\beta\cos\varphi)=0 \tag{104}$$

for the mean range $(1/\beta)$ of the short-range correlation in the direction φ, when $H'<H^*$.

THERMODYNAMIC PROPERTIES OF A LARGE CRYSTAL

To compute the partition function per atom

$$\lambda=\lambda_\infty=\lim_{n=\infty}(\lambda_{\max})^{1/n} \tag{105}$$

for an infinite crystal we replace the sum (95) by the integral

$$\log\lambda_\infty=\tfrac{1}{2}\log(2\sinh 2H)+\frac{1}{2\pi}\int_0^\pi\gamma(\omega)d\omega \tag{106}$$

where

$$\cosh\gamma(\omega)=\cosh 2H'\cosh 2H^*-\sinh 2H'\sinh 2H^*\cos\omega.$$

There are several ways to show that (106) actually describes a symmetrical function of H and H'. For example, with the aid of the useful identity

$$\int_0^{2\pi}\log(2\cosh x-2\cos\omega)d\omega=2\pi x \tag{107}$$

we can convert (106) into the double integral

$$\log(\lambda/2)=\tfrac{1}{2}\pi^{-2}\int_0^\pi\int_0^\pi\log(\cosh 2H\cosh 2H'-\sinh 2H\cos\omega-\sinh 2H'\cos\omega')d\omega d\omega'. \tag{108}$$

It seems rather likely that this result could be derived from direct algebraic and topological considerations without recourse to the operator

method used in the present work. Such a development might well amount to a great improvement of the theory.

A generalization of the expansion whose initial terms were given by Kramers and Wannier is easily obtained from (108). With the notation

$$\begin{aligned} 2\kappa &= \tanh 2H/\cosh 2H' = \sin g \cos g', \\ 2\kappa' &= \tanh 2H'/\cosh 2H = \cos g \sin g' \end{aligned} \tag{109a}$$

we expand the logarithm in powers of κ and κ' and integrate term by term to obtain

$$\begin{aligned} &\log \lambda - \tfrac{1}{2}\log(4\cosh 2H \cosh 2H') \\ &= \tfrac{1}{2}\pi^{-2}\int_0^\pi\int \log(1-2\kappa\cos\omega - 2\kappa'\cos\omega')d\omega d\omega' \\ &= -\tfrac{1}{2}\sum_{r+s>0}(2r+2s-1)!(r!)^{-2}(s!)^{-2}\kappa^{2r}\kappa'^{2s}. \end{aligned} \tag{109b}$$

Specialization to the case $H=H'$; $\kappa=\kappa'$ of quadratic symmetry yields

$$\begin{aligned} &\log\lambda - \log(2\cosh 2H) \\ &= \tfrac{1}{2}\pi^{-2}\int_0^\pi\int \log(1-4\kappa\cos\omega_1\cos\omega_2)d\omega_1 d\omega_2 \\ &= -\sum_{n=1}^{\infty}\left(\binom{2n}{n}^2/4n\right)\kappa^{2n} \\ &= \log(1-\kappa^2-4\kappa^4-29\kappa^6-265\kappa^8-2745\kappa^{10} \\ &\qquad -30773\kappa^{12}-364315\kappa^{14}-\cdots) \end{aligned} \tag{109c}$$

which confirms the result given previously to the order κ^{10} by Kramers and Wannier.[10]

These expansions converge for all values of H and H' because

$$|2\kappa\cos\omega + 2\kappa'\cos\omega'| \leqq 2\kappa+2\kappa' = \sin(g+g') \leqq 1.$$

The limit of convergence of the series is given by the transition point,[18] and it converges even at the limit. Of course it is not very suitable for computation in the critical region; much better formulas for this purpose will be obtained.

The partition function (106) yields directly the free energy F of the crystal; the energy U and the specific heat C are obtained by differentiation with regard to the temperature T.

[18] Kramers and Wannier might well have inferred this much from the uniform sign of the terms, which locates the nearest singularity on the real axis.

For a crystal of N atoms

$$\begin{aligned} F &= U - TS = -NkT\log\lambda, \\ U &= F - T(dF/dT) = NkT^2 d(\log\lambda)/dT, \\ C &= dU/dT. \end{aligned} \tag{110}$$

For the purpose of differentiation it will be convenient to consider λ, given by (106), as a function of two independent variables $H=J/kT$ and $H'=J'/kT$. In this notation we have

$$\begin{aligned} U &= -NJ(\partial\log\lambda/\partial H) - NJ'(\partial\log\lambda/\partial H') \\ &= -NkT(H(\partial\log\lambda/\partial H) \\ &\qquad + H'(\partial\log\lambda/\partial H')) \end{aligned} \tag{111a}$$

$$\begin{aligned} C = Nk(&H^2(\partial^2\log\lambda/\partial H^2) \\ &+ 2HH'(\partial^2\log\lambda/\partial H\partial H') \\ &+ H'^2(\partial^2\log\lambda/\partial H'^2)). \end{aligned} \tag{111b}$$

The two terms of (111a) are separately the mean energies of interaction in the two perpendicular directions in the crystal (remember the interpretation of temperature as a statistical parameter).

In differentiating the integral of (106) we consider H^* as a function of H which satisfies [cf. (17)]

$$dH^*/dH = -\sinh 2H^* = -1/\sinh 2H.$$

The following formulas, wherein γ, δ', and δ^* are considered as functions of H', H^*, and ω, are easily obtained by differentiation from the formulas (89); some of them are obvious by inspection of Fig. 4.

$$\begin{aligned} \partial\gamma/\partial H' &= 2\cos\delta^*, \\ \partial\gamma/\partial H^* &= 2\cos\delta', \\ \partial^2\gamma/\partial H'^2 &= 4\sin^2\delta^*\coth\gamma, \\ \partial^2\gamma/\partial H^{*2} &= 4\sin^2\delta'\coth\gamma, \\ \partial^2\gamma/\partial H'\partial H^* &= -4\sin\delta^*\sin\delta'/\sinh\gamma. \end{aligned} \tag{112}$$

Comparison with (106) yields for substitution in (111)

$$\begin{aligned} \partial\log\lambda/\partial H' &= \int_0^\pi \cos\delta^*\, d\omega/\pi, \\ \partial\log\lambda/\partial H &= \cosh 2H^* - \sinh 2H^*\int_0^\pi \cos\delta'\, d\omega/\pi \end{aligned} \tag{113a}$$

and

$$\partial^2\log\lambda/\partial H'^2 = 2\int_0^\pi \sin^2\delta^*\coth\gamma\, d\omega/\pi,$$

$$\partial^2 \log \lambda/\partial H \partial H' = 2 \sinh 2H^* \times \int_0^\pi (\sin \delta^* \sin \delta'/\sinh \gamma) d\omega/\pi,$$
$$\partial^2 \log \lambda/\partial H^2 = 2 \sinh^2 2H^* \times \Big(-1+\coth 2H^* \int_0^\pi \cos \delta' \, d\omega/\pi + \int_0^\pi \sin^2 \delta' \coth \gamma \, d\omega/\pi\Big). \quad (113b)$$

The reduction of these integrals by means of an uniformizing elliptic substitution for the hyperbolic triangle of Fig. 4 is dealt with in the appendix. The qualitative behavior of the integrals is easily seen from Fig. 4: The integrals (113a) are continuous functions of H' and H (or H^*) for all values of these parameters, even for $H'=H^*$ (critical point). The three integrals (113b) are infinite at the critical point, otherwise finite. The singularity results from a conspiracy: In the case $H'=H^*$ we have $\gamma(0)=0$ and at the same time $\delta'(0)=\delta^*(0)=\frac{1}{2}\pi$, although at all other temperatures

$$\gamma(\omega) \gtreqless \gamma(0) = 2|H'-H^*| > 0,$$
$$\sin \delta'(0) = \sin \delta^*(0) = \sin 0 = \sin \pi = 0.$$

For the special case of quadratic symmetry $H'=H$ the computation of the thermodynamic functions can be simplified considerably. The most convenient starting point is the double integral of (109c), which is converted into a single integral with the aid of (107). Using the notation

$$k_1 = 4\kappa = 2 \sinh 2H/\cosh^2 2H, \quad k_1'' = \pm(1-k_1^2)^{\frac{1}{2}} = 2\tanh^2 2H - 1; \quad |k_1''| = k_1' \quad (114)$$

we obtain

$$\log(\lambda/2\cosh 2H) = \frac{1}{2\pi}\int_0^\pi \log(\tfrac{1}{2}(1+(1-k_1^2 \sin^2 \varphi)^{\frac{1}{2}}))d\varphi. \quad (115)$$

Differentiation under the integral sign yields for the energy U,

$$U = -NJ\frac{d \log \lambda}{dH} = -NJ \coth 2H\Big(1+\frac{2}{\pi}k_1'' K_1\Big) \quad (116)$$

and for the specific heat C,

$$C = Nk\frac{d^2 \log \lambda}{dH^2} = Nk(H \coth 2H)^2(2/\pi) \times (2K_1 - 2E_1 - (1-k_1'')(\tfrac{1}{2}\pi + k_1'' K_1)). \quad (117)$$

In these formulas K_1 and E_1 denote the complete elliptic integrals

$$K_1 = K(k_1) = \int_0^{\pi/2} (1-k_1^2 \sin^2 \varphi)^{-\frac{1}{2}} d\varphi,$$
$$E_1 = E(k_1) = \int_0^{\pi/2} (1-k_1^2 \sin^2 \varphi)^{\frac{1}{2}} d\varphi. \quad (118a)$$

The integral (115) cannot be expressed in closed form; but rapidly convergent series can be given. With the notation

$$K_1' = K(k_1'), \quad \log q_1 = \pi\tau_1 i = -\pi K_1'/K_1, \quad (118b)$$
$$G = 1^{-2} - 3^{-2} + 5^{-2} - 7^{-2} + \cdots = 0.915\,965\,594 \text{ (Catalan's constant)},$$

one or the other of the following expansions (derived in the appendix) will be found suitable for computation:

$$\log \lambda = \tfrac{1}{2}\log(2\sinh 2H) - \tfrac{1}{4}\log q_1 + \sum_{n=1}^{\infty} (-)^n (2n-1)\log(1-q_1^{2n-1}), \quad (119a)$$

$$\log \lambda = \tfrac{1}{2}\log(2\sinh 2H) + (2/\pi)G + \frac{1}{\pi}\sum_{n=0}^{\infty}(-)^n \times \frac{(1+(2n+1)(\pi i/\tau_1) - \exp[-(2n+1)\pi i/\tau_1])}{(2n+1)^2 \sinh^2((n+\frac{1}{2})\pi i/\tau_1)}. \quad (119b)$$

A singularity occurs for $H=H^*=\frac{1}{2}\log\cot \pi/8$, in which case $k_1=1$; $K_1=\infty$; $K_1'=\frac{1}{2}\pi$; $E_1=1$. The specific heat becomes infinite at this critical point; the energy is continuous because $k_1''=0$. The analytic nature of the singularity is evident from the approximate formulas

$$K_1 \sim \log(4/k_1') \sim \log(2^{\frac{1}{2}}/|H-H_c|),$$
$$C/Nk \sim (2/\pi)(\log\cot \pi/8)^2(K_1 - 1 - \tfrac{1}{4}\pi). \quad (120)$$

The critical data are

$$H_c = J/kT_c = \tfrac{1}{2}\log\cot\pi/8 = 0.440\ 686\ 8,$$
$$-F_c/NkT_c = \log\lambda_c = \tfrac{1}{2}\log 2 + (2/\pi)G = 0.929\ 695\ 40, \quad (121)$$
$$-U_c/NJ = 2^{\frac{1}{2}} = 1.414\ 213\ 56,$$
$$S_c/Nk = \log\lambda_c - 2^{\frac{1}{2}}H_c = 0.306\ 470 = \log 1.358\ 621.$$

The critical temperature and energy were given already by Kramers and Wannier.[10] In addition, their estimate of "about 2.5335" for λ_c was very close to the exact value

$$\lambda_c = 2^{\frac{1}{8}}e^{2G/\pi} = 2.533\ 737\ 28.$$

The specific heat of a quadratic crystal is represented in Fig. 6 as a function of $1/H = (k/J)T$; the result of the best approximate computation in the literature[10] is indicated for comparison.

Figure 7 represents the specific heat curve of a highly anisotropic crystal ($J'/J = 1/100$), computed from Eq. (6.2) in the Appendix. The corresponding curves for the case of quadratic symmetry ($J'/J = 1$) and for the linear chain ($J'/J = 0$) are also shown. The abscissa is $2/(H+H') = 2kT/(J+J')$, so that the three curves have the same area.

SOME PROPERTIES OF FINITE CRYSTALS

The partition function of any *finite* crystal is an analytic function of the temperature. Perfect order and a sharp transition point occur only when the extent of the crystal is infinite in two directions. It is a matter of interest to study the approach to complete order and the sharpening of the transition point with increasing size (width) of the crystal.

Boundary Tension

First, let us compute the "boundary tension" between two regions of opposite order below the transition point. This we can do by a slight variation of the model. We simply chose a *negative* interaction energy between adjacent atoms in the same tier:

$$u = +J'\sum_1^n \mu_j\mu_{j+1}.$$

Now if n is *even*, the reversal of J' has the same trivial effect as a redefinition of the sign of every other μ_j. The interpretation of the result is a little different in that the type of order which occurs below the transition point is now a superlattice with the ideal structure indicated by Fig. 8. However, let us choose an *odd* value of n. Now a perfect alternation of signs around the polygon of n atoms is impossible; in one place at least the given superlattice must be adjacent to one of opposite order. As we build a long crystal on the odd polygonal base, we build it with one misfit "seam." The free energy difference due to this seam will equal that of a boundary between regions of opposite order.

The formula (93) is still valid, only now

$$J'/kT = -H' > H^* > 0$$

whence

$$\log\lambda_{\max} - \tfrac{1}{2}n\log(2\sinh 2H) = \gamma_1+\gamma_3+\cdots+\gamma_{2m-1}-(|H'|-H^*) = \gamma_1+\gamma_3+\cdots+\gamma_{2m-1}+\tfrac{1}{2}\gamma_{2m+1}-2(|H'|-H^*)$$

where

$$\cosh\gamma_r = \cosh 2H'\cosh 2H^* - \sinh(-2H')\sinh 2H^*\cos(\pi-\omega_r).$$

The replacement of ω_r by $\pi-\omega_r$ has no appreciable effect on the sum; the modification of the partition function due to the seam is therefore practically equal to

$$-2|H'|+2H^*.$$

This represents the effect of a lengthwise boundary for our original model as well, and we obtain

$$\sigma'/kT = -\log\lambda_b' = 2(H'-H^*), \qquad \sigma' = 2J' - kT\log\coth(J/kT) \quad (122a)$$

for the boundary tension σ' (per atom) of a longitudinal boundary. The transverse boundary tension σ is similarly given by

$$\sigma/kT = -\log\lambda_b = 2(H-H'^*). \quad (122b)$$

The boundary tensions both vanish at the critical point, as one should expect. The formulas

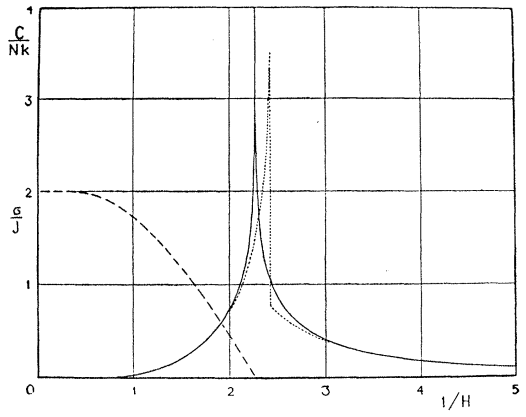


FIG. 6. Properties of quadratic crystal. — — — — — — Boundary tension σ between regions of opposite order. ———— Specific heat C. - - - - - - - - - - - - Approximate computation of C by Kramers and Wannier.

for the boundary entropies and energies follow

$$\begin{aligned} s_b' &= -d\sigma'/dT = 2k((H/\sinh 2H)+H^*), \\ s_b &= -d\sigma/dT = 2k((H'/\sinh 2H')+H'^*), \\ u_b' &= \sigma'+Ts_b' = (2/\sinh 2H)J+2J', \\ u_b &= \sigma+Ts_b = 2J+(2/\sinh 2H')J'. \end{aligned} \tag{123}$$

The variation of σ with the temperature for a quadratic crystal ($J=J'$) is represented graphically in Fig. 6.

Mean Ordered Length

In a crystal of moderate width n we may expect to find sections of rather well-defined order similar to that of an infinite crystal, with occasional transitions to opposite order. The result (122b) allows an estimate of the "mean ordered length" l_0 between such interruptions. By the general theory of fluctuations

$$\begin{aligned} l_0 = \lambda_b^{-n} &= \exp[2n(H-H'^*)] \\ &= (e^{2H}\tanh H')^n. \end{aligned} \tag{124}$$

Evidently, when n is large enough we have

$$l_0 \gg n.$$

The estimate (124) is significant when this condition is fulfilled.

The Specific Heat of a Finite Crystal

Since the partition function of a finite crystal is an analytic function of the temperature, its specific heat will be finite at all temperatures. However, a maximum will occur near the transition point of the infinite crystal; this maximum will be increased and sharpened with increasing size of the crystal.

Kramers and Wannier[10] computed the specific heats at the transition point successively for $n=1, 2, \cdots, 6$ (screw arrangement). From the results they inferred the asymptotic rule that the height of the maximum increases linearly with $\log n$. We shall verify this remarkable conjecture.

The maximum of (C/N) for a finite crystal does not occur exactly at the asymptotic critical point; but the differences in location and magnitude are only of the order $n^{-2}\log n$. This order of accuracy will suffice.

To compute the specific heat we substitute the exact partition function (95) of a finite crystal in (111b), whereby the relations (112) are useful. The specialization to the critical case

$$H'=H^*; \quad \text{gd } 2H+\text{gd } 2H'=\tfrac{1}{2}\pi; \quad \sinh 2H \sinh 2H'=1$$

simplifies the computation in several respects; the relations

$$\delta'=\delta^*=\delta, \quad \sinh\tfrac{1}{2}\gamma = \sinh 2H' |\sin\tfrac{1}{2}\omega|$$

are valid in this case. We write the result in the form

$$\begin{aligned} C/Nk = &-2H^2\sinh^2 2H'+(H'+H\sinh 2H')^2 \\ &\times\sinh 2H\times\frac{1}{n}\sum_{r=1}^{n}\operatorname{cosec}[(r-\tfrac{1}{2})\pi/n) \\ &+\frac{1}{n}\sum_{r=1}^{n}[(H'+H\sinh 2H')^2 \\ &\times(2\sin^2\delta_{2r-1}\coth\gamma_{2r-1}-\operatorname{cosech}\tfrac{1}{2}\gamma_{2r-1}) \\ &-4HH'\sinh 2H'\sin^2\delta_{2r-1}\tanh\tfrac{1}{2}\gamma_{2r-1} \\ &+H^2\sinh 4H'\cos\delta_{2r-1}]. \end{aligned} \tag{125}$$

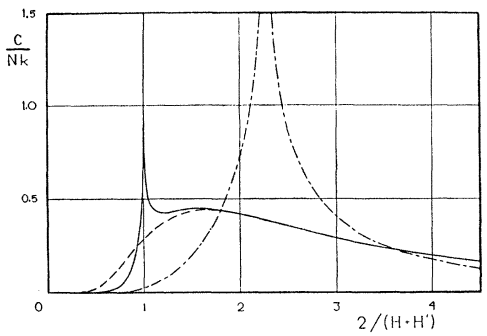


FIG. 7. Specific heats for varying degrees of anisotropy. ———— $J'/J=1/100$; — — — — — — — $J'/J=1$ (quadratic crystal); - - - - - - $J'=0$ (linear chain).

The second summand, when considered as a periodic function of the variable $\omega_{2r-1}=(2r-1)\pi/2n$, has a differential quotient of bounded variation. Its sum may be replaced accordingly by the corresponding integral, with an error of the order n^{-2}.

We have purposely split off the first sum

$$S_1=\frac{1}{n}\sum_{r=1}^{n}\operatorname{cosec}((r-\tfrac{1}{2})\pi/n).$$

The corresponding integral diverges. For an asymptotic estimate of the sum we expand the cosecants in partial fractions; the result is easily arranged in the form

$$S_1=\frac{4}{\pi}\left(\frac{1}{1}+\frac{1}{3}+\cdots+\frac{1}{2n-1}-\frac{1}{2n+1}-\frac{1}{2n+3}-\cdots-\frac{1}{4n-1}+\frac{1}{4n+1}+\cdots\right)$$
$$=\frac{2}{\pi}\sum_{m=0}^{\infty}(-)^m(\psi((m+1)n+\tfrac{1}{2})-\psi(mn+\tfrac{1}{2}))$$

whereby

$$\psi(z)\equiv\Gamma'(z)/\Gamma(z)=\log(z-\tfrac{1}{2})+O(z^{-2}).$$

From the given asymptotic estimate of $\psi(z)$ together with

$$\psi(\tfrac{1}{2})=-2\log 2-C_E,$$
$$C_E=0.577\ 215\ 665,\quad\text{(Euler's constant)}$$
$$\log\left(\frac{2}{1}\cdot\frac{2}{3}\cdot\frac{4}{3}\cdot\frac{4}{5}\cdot\cdots\right)=\log\frac{\pi}{2},\quad\text{(Wallis' product)}$$

we obtain

$$S_1=(2/\pi)(\log(8n/\pi)+C_E)+O(n^{-2}).$$

Substitution of the given estimates in (125) yields the asymptotic formula for the specific heat maximum

$$C/Nk\sim(2/\pi)[\sinh 2H(H'+H\sinh 2H')^2\times(\log n+\log(8/\pi\cosh 2H')+C_E)+\sinh 2H(H'-H\sinh 2H')^2-2(H'\sinh 2H)^2\,\mathrm{gd}\,2H'-2(H\sinh 2H')^2\,\mathrm{gd}\,2H].\quad(126)$$

The result is not quite symmetrical with regard to H and H'; neither was such symmetry to be expected. Interchange of the two leads to the replacement

$$\log(n/\cosh 2H')\rightarrow\log(n/\cosh 2H).$$

For the case of quadratic symmetry

$$H=H'=\tfrac{1}{2}\log\cot\pi/8$$

the coefficient of $\log n$ attains a maximum. We find

$$C/Nk\sim(2/\pi)(\log\cot\pi/8)^2\times(\log n+\log(2^{5/2}/\pi)+C_E-\tfrac{1}{4}\pi)$$
$$=0.4945\log n+0.1879.\quad(127)$$

The estimate indicated graphically by Kramers and Wannier[10] may be described by the equation

$$C/Nk=0.48\log n+0.21.$$

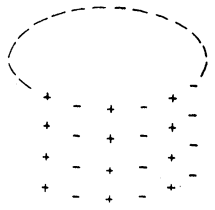


FIG. 8. Superlattice at low temperatures in crystal for which the interaction energy between neighbors of opposite spin is $J>0$ lengthwise and $-J'<0$ transversely.

APPENDIX

We shall deal here with the evaluation of various integrals which occur in the text. Most of these can be reduced in straightforward fashion to complete elliptic integrals; only the partition function itself is of a type one step higher than the theta functions, and involves a little analysis which is not found in textbooks.

1. General Notation

One of the main reasons for setting this material apart is that the notation must be specified because there are several systems in common use. We shall adopt the notation used by Whitaker and Watson.[19]

[19] E. T. Whitaker and G. N. Watson, *Modern Analysis* (Cambridge University Press, 1927), fourth edition, Chapters 20–22. Referred to in the following as WW.

Theta Functions

$$\vartheta_3(z|\tau)=\vartheta_3(z)=\vartheta_4(z+\tfrac{1}{2}\pi)$$
$$=\sum_{-\infty}^{\infty}\exp(n^2\pi i\tau)\cos 2nz,$$
$$\vartheta_2(z|\tau)=\vartheta_2(z)=\vartheta_1(z+\tfrac{1}{2}\pi)$$
$$=\sum_{-\infty}^{\infty}\exp[(n+\tfrac{1}{2})^2\pi i\tau]\cos(2n+1)z, \tag{1.1}$$
$$\vartheta_r=\vartheta_r(0);\quad \vartheta_r''=\vartheta_r''(0);\quad (r=2,3,4).$$

Periods, Modulus, Comodulus

$$2K=\vartheta_3^2\pi;\quad 2iK'=\vartheta_3^2\pi\tau,$$
$$k=\sin\theta=\vartheta_2^2/\vartheta_3^2,$$
$$k'=\cos\theta=\vartheta_4^2/\vartheta_3^2, \tag{1.2}$$
$$\log q=\pi i\tau=-\pi K'/K.$$

We shall only have to deal with "natural" cases in which $-i\tau$ is real (not negative); $0<k\leqq 1$; $0\leqq k'<1$. The ratio τ of the periods will be specified when necessary. Tables of $\log q$ are available.[20]

Jacobian Elliptic Functions

$$\operatorname{sn}(\vartheta_3^2 z)=(\vartheta_3/\vartheta_2)\vartheta_1(z)/\vartheta_4(z),$$
$$\operatorname{cn}(\vartheta_3^2 z)=(\vartheta_4/\vartheta_2)\vartheta_2(z)/\vartheta_4(z),$$
$$\operatorname{dn}(\vartheta_3^2 z)=(\vartheta_4/\vartheta_3)\vartheta_3(z)/\vartheta_4(z), \tag{1.3}$$
$$\operatorname{am} u=\sin^{-1}(\operatorname{sn} u)=\cos^{-1}(\operatorname{cn} u).$$

We shall use Glaisher's notation for the quotients of the Jacobian elliptic functions

$$\operatorname{sc} u=\operatorname{sn} u/\operatorname{cn} u;\quad \operatorname{nd} u=1/\operatorname{dn} u;\quad \text{etc.} \tag{1.4}$$

The Functional Relations

$$\operatorname{cn}^2 u+\operatorname{sn}^2 u=\operatorname{dn}^2 u+k^2\operatorname{sn}^2 u=1 \tag{1.5}$$

are important for the uniformization of certain algebraic functions.

Elliptic Integrals of the First Kind

$$d(\operatorname{sn} u)/du=\operatorname{cn} u\operatorname{dn} u;\quad \text{etc.}$$
$$u=F(k,\operatorname{am} u)=\int_0^{\operatorname{am} u}(1-k^2\sin^2\varphi)^{-\frac{1}{2}}d\varphi, \tag{1.6}$$
$$K(k)=F(k,\tfrac{1}{2}\pi);\quad K'(k)=K(k').$$

[20] Four place tables of $\log q$ by 5′ intervals of the modular angle are given by E. Jahnke and F. Emde, *Tables of Functions* (B. G. Teubner, Leipzig and Berlin, 1933), second edition, p. 122.

Elliptic Integrals of the Second Kind

These involve the following definitions and relations.

$$Z(u)=\vartheta_3^{-2}\vartheta_4'(\vartheta_3^{-2}u)/\vartheta_4(\vartheta_3^{-2}u),$$
$$E=\int_0^{\pi/2}(1-k^2\sin^2\varphi)^{\frac{1}{2}}d\varphi$$
$$=\int_0^K \operatorname{dn}^2 u\,du=(-\vartheta_2''/\vartheta_2\vartheta_3^2)\pi/2, \tag{1.7}$$
$$E(u)=Z(u)+(E/K)u=\int_0^u \operatorname{dn}^2 v\,dv.$$

Complete Elliptic Integral of the Third Kind

$$KZ(a)=\int_0^K k^2\operatorname{sn} a\operatorname{cn} a\operatorname{dn} a\operatorname{sn}^2 u$$
$$\times(1-k^2\operatorname{sn}^2 a\operatorname{sn}^2 u)^{-1}du. \tag{1.8}$$

2. Uniformizing Substitution

The trigonometric functions of the angles and sides of a spherical triangle with two fixed parts can always be expressed in terms of single-valued functions by a suitable elliptic substitution. The same is true for hyperbolic (and plane) triangles. In any case the determination of the modulus is suggested by the sine proportion.

For the triangle of Fig. 4, with two given sides $2H'$ and $2H^*$, the simplest uniformizing substitution depends on which side is longer. For temperatures below the critical point we choose the modulus k, the imaginary parameter ia, and the new variable u as follows

$$k=k_0=\sin\Theta_0=\sinh 2H^*/\sinh 2H'$$
$$=1/\sinh 2H\sinh 2H'<1,$$
$$\operatorname{am}(ia)=\operatorname{am}(2iK_0'y,k_0)=2iH', \tag{2.1a}$$
$$\operatorname{am} u=\delta'.$$

Then the trigonometric, *viz.*, hyperbolic functions of δ^*, δ', $2H^*$ and $2H'$ are given by the formulas

$$\sin\delta'=\operatorname{sn} u;\quad \sin\delta^*=k\operatorname{sn} u$$
$$\cos\delta'=\operatorname{cn} u;\quad \cos\delta^*=\operatorname{dn} u$$
$$\tan g'=\sinh 2H'=-i\operatorname{sn} ia$$
$$\cot g=\sinh 2H^*=-ik\operatorname{sn} ia \tag{2.2a}$$
$$\sec g'=\cosh 2H'=\operatorname{cn} ia$$
$$\operatorname{cosec} g=\cosh 2H^*=\operatorname{dn} ia.$$

We are using the abbreviation

$$g'=\mathrm{gd}\,2H';\quad g=\mathrm{gd}\,2H=\tfrac{1}{2}\pi-\mathrm{gd}\,2H^* \tag{2.3}$$

for the gudermannian angles, which can often be employed to advantage in numerical computations.

For temperatures above the critical point the starred and the primed quantities exchange roles:

$$\begin{aligned} k=k_0&=\sin\Theta_0=\sinh 2H'/\sinh 2H^*\\ &=\sinh 2H'\sinh 2H=<1,\\ \mathrm{am}(ia)&=\mathrm{am}(2iK_0'y,k_0)=2iH^*,\\ \mathrm{am}\,u&=\delta^* \end{aligned} \tag{2.1b}$$

and explicitly

$$\begin{aligned} \sin\delta'&=k\,\mathrm{sn}\,u;\quad \sin\delta^*=\mathrm{sn}\,u\\ \cos\delta'&=\mathrm{dn}\,u;\quad \cos\delta^*=\mathrm{cn}\,u\\ \tan g'&=\sinh 2H'=-ik\,\mathrm{sn}\,ia\\ \cot g&=\sinh 2H^*=-i\,\mathrm{sn}\,ia\\ \sec g'&=\cosh 2H'=\mathrm{dn}\,ia\\ \mathrm{cosec}\,g&=\cosh 2H^*=\mathrm{cn}\,ia. \end{aligned} \tag{2.2b}$$

The formulas for ω and γ are the same in the two cases. The abbreviation

$$M=\mathrm{dn}\,ia\,\mathrm{dn}\,u-k\,\mathrm{cn}\,ia\,\mathrm{cn}\,u$$

will be convenient; then

$$\begin{aligned} \cosh\gamma&=(\mathrm{cn}\,ia\,\mathrm{dn}\,u-k\,\mathrm{dn}\,ia\,\mathrm{cn}\,u)/M\\ \sinh\gamma&=-ik'^2\,\mathrm{sn}\,ia/M\\ -\cos\omega&=(\mathrm{dn}\,ia\,\mathrm{cn}\,u-k\,\mathrm{cn}\,ia\,\mathrm{dn}\,u)/M\\ \sin\omega&=k'^2\,\mathrm{sn}\,u/M. \end{aligned} \tag{2.4}$$

Moreover, when ω and γ are considered as functions of u and a

$$\begin{aligned} -\partial\omega/\partial u&=\partial\gamma/\partial a=k'^2/M,\\ \partial\gamma/\partial u&=\partial\omega/\partial a=ik'^2k\,\mathrm{sn}\,ia\,\mathrm{sn}\,u/M. \end{aligned} \tag{2.5}$$

The conformal mapping indicated by (2.5) may be described by the functional relation

$$\cot\tfrac{1}{2}(\omega-i\gamma)=(1+k)\,\mathrm{sc}\,\tfrac{1}{2}(u+ia)\,\mathrm{nd}\,\tfrac{1}{2}(u+ia). \tag{2.6}$$

3. Alternative Substitution

While the substitution given above is preferred for most purposes, there are certain advantages to be gained by a Landen transformation to modulus and periods given by

$$\begin{aligned} k_1'&=\cos\Theta_1=\coth(H'+H^*)\tanh|H'-H^*|\\ &=|\cos(g+g')|/\cos(g-g')=(1-k_0)/(1+k_0),\\ k_1&=\sin\Theta_1=2(\sinh 2H\sinh 2H')^{\frac{1}{2}}/\\ &\qquad(1+\sinh 2H\sinh 2H'),\\ K_1&=(1+k_0)K_0,\\ K_1'&=\tfrac{1}{2}(1+k_0)K_0'=K_0'/(1+k_1'),\\ \tau_1&=iK_1'/K_1=\tfrac{1}{2}\tau_0=\tfrac{1}{2}\tau. \end{aligned} \tag{3.1}$$

The parameter

$$ia_1=2yiK_1'=\tfrac{1}{2}(1+k_0)ia_0 \tag{3.2}$$

and the variable u_1 are given by

$$\begin{aligned} \mathrm{am}(ia_1,k_1)&=i(H'+H^*),\\ \mathrm{am}(u_1,k_1)&=\tfrac{1}{2}(\delta'+\delta^*) \end{aligned} \tag{3.3}$$

and the following relations hold

$$\begin{aligned} \mathrm{am}(K_1-ia_1)&=\tfrac{1}{2}\pi-i|H'-H^*|,\\ \mathrm{am}(K_1-u_1)&=\tfrac{1}{2}\pi-\tfrac{1}{2}|\delta'-\delta^*|,\\ \mathrm{am}(u_1\pm ia_1)&=\tfrac{1}{2}(\pi-\omega\pm i\gamma). \end{aligned} \tag{3.4}$$

Here the functions of the double parameter are of some interest

$$\begin{aligned} \mathrm{sc}(2ia_1)&=\mathrm{sc}(4iyK_1')=i\cos(g-g'),\\ \mathrm{nc}(2ia_1)&=\mathrm{nc}(4iyK_1')=\sin(g-g'),\\ \mathrm{dc}(2ia_1)&=\mathrm{dc}(4iyK_1')=\sin(g+g'). \end{aligned} \tag{3.5}$$

This substitution shows up the analytic nature of the parameter through the critical point, and (2.6) is replaced by a simpler equivalent in (3.4). Moreover, formulas valid for all temperatures can be constructed by furnishing a sign for the comodulus

$$\begin{aligned} k_1'&=|k_1''|;\\ k_1''&=\coth(H'+H^*)\tanh(H'-H^*). \end{aligned} \tag{3.6}$$

That advantage together with the previous usage of Kramers and Wannier[10] decided the choice of elliptic substitution in the text.

4. Discussion of the Parameter

The imaginary parameter ia given by (2.1) can be evaluated as a real elliptic integral of the first kind. For that purpose we use Jacobi's imaginary transformation, described by the

relations

$$i\,\mathrm{cs}(iu,k)\,\mathrm{sn}(u,k')=\mathrm{cn}(iu,k)\,\mathrm{cn}(u,k')$$
$$=\mathrm{dn}(iu,k)\,\mathrm{cd}(u,k')=1 \quad (4.1)$$

and the parameter can be determined by the formula

$$\mathrm{am}(a_0,k_0')=\mathrm{am}(2yK_0',k_0')=\mathrm{gd}\,2H'=g',$$
$$a_0=2yK_0'=F(\cos\Theta_0,g'). \quad (4.2)$$

In tables this elliptic integral is often denoted by $F(90°-\Theta_0,g')$. Alternative formulas can be obtained by Landon transformations, whereby the "elliptic angle" πy is invariant. From (3.4) and (3.5) we obtain, respectively,

$$\mathrm{am}(a_1,\cos\Theta_1)=\mathrm{am}(2yK_1',k_1')$$
$$=\mathrm{gd}(H'+H^*), \quad (4.3)$$
$$\mathrm{am}(2a_1,\cos\Theta_1)=\mathrm{am}(4yK_1',k_1')$$
$$=\tfrac{1}{2}\pi-g+g'. \quad (4.4)$$

Further Landen transformations are best described by the quotients of theta functions. The following are suitable for temperatures not too far removed from the critical point

$$\tan^2\tfrac{1}{2}\Theta_2=\sin\Theta_1$$
$$=(\tan 2g\tan 2g')^{\frac{1}{2}}/\cos(g-g'), \quad (4.5a)$$
$$(\cos\Theta_2)^{\frac{1}{2}}\,\mathrm{sn}(a_2,\cos\Theta_2)$$
$$=\frac{\vartheta_1(2\pi y|-4/\tau)}{\vartheta_4(2\pi y|-4/\tau)}=\frac{\sinh|H'-H^*|}{\cosh(H'+H^*)}$$
$$=|\tan\tfrac{1}{2}(g+g'-\tfrac{1}{2}\pi)|, \quad (4.5b)$$
$$(\cos\Theta_2)^{\frac{1}{2}}\,\mathrm{sn}(2a_2,\cos\Theta_2)=\frac{\vartheta_1(4\pi y|-4/\tau)}{\vartheta_4(4\pi y|-4/\tau)}$$
$$=\sin(g-g')\,|\cot(g+g')|. \quad (4.5c)$$

For temperatures not too close to the critical point we may take

$$k_{-1}=\sin\Theta_{-1}=\tan^2\tfrac{1}{2}\theta_0, \quad (4.6a)$$

and the theta series involved in the following formula (imaginary argument) will converge rapidly:

$$-ik_{-1}^{\frac{1}{2}}\,\mathrm{sn}(iyK_{-1}',k_{-1})=\frac{\vartheta_1(\pi\tau y|2\tau)}{i\vartheta_4(\pi\tau y|2\tau)}$$
$$=\begin{cases}e^{-2H}; & (H'>H^*)\\ \tanh H'; & (H'<H^*).\end{cases} \quad (4.6b)$$

One or the other of the two formulas (4.5) and (4.6) will yield at least 3 significant figures per term of the theta series. When a table of $\log q$ is available (a table of complete elliptic integrals will do), it is not necessary to evaluate θ_2 or Θ_{-1} explicitly.

As regards the variation of the parameter a with the temperature, we note first of all that

$$y=a_0/2K_0'=a_1/2K_1'$$

is analytic at the critical point. This is evident from (3.1) and (3.3); the elliptic integrals which determine a_1 and K_1' are analytic functions of $\cos^2\Theta_1$, which has no singularity there. In this sense the singularities of the various functions at the critical point are completely described by the degeneration of the period parallelogram

$$i/\tau=K/K'=\infty; \quad (H'=H^*).$$

For extreme temperatures, with

$$H=J/kT; \quad H'=J'/kT$$

the asymptotic estimates

$$\lim_{T=0}(2y)=H'/(H+H')=J'/(J+J'),$$
$$\lim_{T=\infty}(2y)=\tfrac{1}{2} \quad (4.7)$$

can be derived from (2.1).

The parameter is an unsymmetrical function of H and H'; the nature of the asymmetry is evident from either of the formulas (4.4) and (4.5c), which involve the double parameter: Interchanging the roles of H and H' replaces y by $\frac{1}{2}-y$, and the parameter ia_0 is replaced by its elliptic complement $i(K_0'-a_0)$. Thus (2.1a) and (2.1b) have the counterparts

$$\mathrm{am}(iK'-ia,k_0)=\mathrm{am}(iK_0'(1-2y),k_0)$$
$$=\begin{cases}2iH; & (H'>H^*)\\ 2iH'^*; & (H'<H^*).\end{cases} \quad (4.8)$$

It is evident that if $J'<J$, we shall have

$$y<\tfrac{1}{4}; \quad a<\tfrac{1}{2}K'; \quad (J'<J) \quad (4.9)$$

for all temperatures, and in the special case of quadratic symmetry

$$y=\tfrac{1}{4}; \quad a=\tfrac{1}{2}K'; \quad (J=J'). \quad (4.10)$$

This is the reason why the results for that case

can be expressed by the complete integrals $K(k)$ and $E(k)$ alone, as given in the text.

5. Reduction of Integrals

By the substitution (2.2), the integrals of (113) in the text are readily evaluated as complete elliptic integrals. For example,

$$\int_0^\pi \cos\delta' d\omega = \int_0^{2K} k'^2 \operatorname{cn} u(\operatorname{dn} ia \operatorname{dn} u - k \operatorname{cn} ia \operatorname{cn} u)^{-1} du; \quad (H'>H^*).$$

If we replace u by $2K-u$, the sign of $\operatorname{cn} u$ is changed; that of $\operatorname{dn} u$ is preserved. Accordingly, that part of the integrand which is odd with regard to $\operatorname{cn} u$ may be omitted, which yields

$$\frac{k \operatorname{cn} ia \operatorname{cn}^2 u}{1-k^2 \operatorname{sn}^2 ia \operatorname{sn}^2 u} = k \operatorname{cn} ia - \frac{k \operatorname{cn} ia \operatorname{dn}^2 ia \operatorname{sn}^2 u}{1-k^2 \operatorname{sn}^2 ia \operatorname{sn}^2 u}$$

whence

$$\int_0^\pi \cos\delta' d\omega = 2K(k \operatorname{cn} ia - k^{-1} \operatorname{ds} ia\, Z(ia)); \quad (H'>H^*).$$

The other integrals (113) are treated similarly. The results are

$$\begin{aligned}
&\int_0^\pi \cos\delta^* d\omega = -2iK(k \operatorname{sn} ia \coth 2H^* - Z(ia) \coth 2H'),\\
&\int_0^\pi \cos\delta' d\omega = -2iK(k \operatorname{sn} ia \coth 2H' - Z(ia) \coth 2H^*),\\
&\int_0^\pi (\sin\delta^* \sin\delta'/\sinh\gamma) d\omega = 2(K-E)(i/k \operatorname{sn} ia),\\
&\sinh^2 2H' \int_0^\pi \sin^2\delta^* \coth\gamma\, d\omega = \sinh^2 2H^* \int_0^\pi \sin^2\delta' \coth\gamma\, d\omega = -2iKZ(ia).
\end{aligned} \tag{5.1}$$

The mixed notation is designed to throw the distinction between the cases (2.2a) and (2.2b) entirely into the choice of modulus and parameter; so that the formulas (5.1) are equally valid for $H'<H^*$ and for $H'>H^*$.

The Z function of imaginary argument which enters into (5.1) can be expressed in terms of the tabulated functions of real argument $Z(a, k')$ as follows:

$$Z(iu, k) = \operatorname{dn}(iu, k) \operatorname{sc}(iu, k) - iZ(u, k') - i(\pi u/2KK'). \tag{5.2}$$

For substitution in (113) it is convenient to make use of the function

$$Z(iK'-ia) = -\operatorname{dn} ia \operatorname{cs} ia - i(\pi/2K) - Z(ia) \tag{5.3}$$

together with $Z(ia)$; this leads to more symmetrical formulas. The connection between the corresponding functions of real argument is

$$Z(a, k') + Z(K'-a, k') = k'^2(-i) \operatorname{sc} ia \operatorname{nd} ia. \tag{5.4}$$

6. Derived Thermodynamic Functions

In assembling the terms of the formula (113a) for the energy it is best to deal with the cases $H'>H^*$ and $H'<H^*$ separately. The results are

$$U = -NJ'(\partial \log\lambda/\partial H') - NJ(\partial \log\lambda/\partial H), \tag{6.1a}$$

$$\partial \log\lambda/\partial H' = \coth 2H'(2y + (2K/\pi)Z(2yK', k')), \quad (H'>H^*) \tag{6.1b}$$

$$\partial \log\lambda/\partial H = \coth 2H \times (1-2y+(2K/\pi)Z((1-2y)K', k'))$$

valid for temperatures below the critical point; above the critical point we have instead

$$\partial \log\lambda/\partial H' = \coth 2H' \times (2y-(2K/\pi)Z((1-2y)K', k')) \quad (H'<H^*). \tag{6.1c}$$

$$\partial \log\lambda/\partial H = \coth 2H \times (1-2y-(2K/\pi)Z(2yK', k'))$$

The energy is continuous at the critical point because, when u is real [cf. (5.4)]

$$0 \leqq Z(u, k') \leqq 1-k.$$

For the specific heat we obtain from (113b) and (5.1), in mixed notation valid for all temperatures

$$\frac{C}{Nk} = \frac{4}{\pi}\left(-iKZ(ia)\left(\frac{H'}{\sinh 2H'}\right)^2 - iKZ(iK'-ia)\left(\frac{H}{\sinh 2H}\right)^2 + 2(K-E)\left(\frac{\operatorname{sn} ia}{i \sinh 2H'}\right)HH'\right). \tag{6.2}$$

Every term is positive. The specific heat is infinite at the critical point, where $k=1$. This is caused by the factor K; the general case is substantially like the special case of quadratic symmetry treated in the text.

7. The Partition Function

To compute the partition function (106) in terms of τ and y we first differentiate under the integral sign

$$\frac{\partial}{\partial a}\int_0^\pi \gamma\, d\omega=\int_0^{2K}\left(-\frac{\partial\gamma}{\partial a}\frac{\partial\omega}{\partial u}-\gamma\frac{\partial^2\omega}{\partial a\partial u}\right)du.$$

Integration by parts yields with the aid of (2.5)

$$\int_0^{2K}\left(-\frac{\partial\gamma}{\partial a}\frac{\partial\omega}{\partial u}+\frac{\partial\gamma}{\partial u}\frac{\partial\omega}{\partial a}\right)du$$
$$=\int_0^{2K}\left(\left(\frac{\partial\gamma}{\partial a}\right)^2+\left(\frac{\partial\gamma}{\partial u}\right)^2\right)du$$
$$=\int_0^{2K}\left(\frac{\mathrm{dn}^2\, ia\ \mathrm{dn}^2\, u+k^2\,\mathrm{cn}^2\, ia\,\mathrm{cn}^2\, u}{1-k^2\,\mathrm{sn}^2\, ia\,\mathrm{sn}^2\, u}\right)du.$$

The integral is easily evaluated; then considering that

$$\gamma(0,u)=\cosh^{-1}(1)=0$$

for $a=0$, we have

$$\int_0^\pi \gamma\, d\omega=2K\int_0^a \Phi(iu)du, \tag{7.1}$$
$$\Phi(u)=2\,\mathrm{dn}^2\, u-k'^2-2\,\mathrm{dn}\, u\,\mathrm{cs}\, u\, Z(u).$$

The function $\Phi(u)$ is even and periodic with the period $2K$. Its singularities are poles at the points

$$u=2mK+niK';\quad (m, n \text{ integers};\ n\neq 0).$$

Jacobi's imaginary transformation (4.1), (5.2) yields

$$\Phi(iu)=-k'^2+\mathrm{dc}(u,k')\,\mathrm{ns}(u,k')\times(2Z(u,k')+(\pi u/KK')). \tag{7.2}$$

Accordingly, the poles of $\Phi(u)$ are simple; the residues are

$$R(2mK+niK')=R(niK')=(-)^n n\pi i/K. \tag{7.3}$$

It is easily seen that $\Phi(u)$ satisfies the standard conditions for development in partial fractions *qua* function of $\cos(\pi u/K)$. The residues (7.3) together with the condition

$$\Phi(K)+\Phi(K+iK')=k'^2-k'^2=0$$

suffice to determine the expansion

$$\Phi(u)=\left(\frac{\pi}{2K}\right)^2\left(1-8\sum_{n=1}^{\infty}(-)^n n\times\frac{(q^n\cos(\pi u/K)-q^{2n})}{(1-2q^n\cos(\pi u/K)+q^{2n})}\right). \tag{7.4}$$

The integration required by (7.1) is readily performed, and the formula (106) of the text becomes

$$-\frac{F}{NkT}=\log\lambda=\tfrac{1}{2}\log(2\sinh 2H)+\frac{1}{2\pi}\int_0^\pi\gamma\, d\omega$$
$$=\tfrac{1}{2}\log(2\sinh 2H)-\tfrac{1}{2}y\log q$$
$$-\sum_{n=1}^{\infty}(-)^n n\log\left(\frac{1-q^{n+2y}}{1-q^{n-2y}}\right). \tag{7.5}$$

Specialization to the case $y=\frac{1}{4}$ yields the formula (119a) of the text, where $q_1^2=q$.

The series of (7.5) converges rapidly except in the immediate neighborhood of the critical point. To obtain an expansion suitable for computation in that region we note from (7.2) that

$$\Phi(iu)-(\pi u/2KK')i\,\mathrm{cs}\, iu\,\mathrm{dn}\, iu$$
$$=2\mathrm{dc}(u,k')\,\mathrm{ns}(u,k')Z(u,k')-k'^2$$

is a periodic function of u with the real period $2K'$. Its Fourier series is easily derived with the aid of the identity

$$K(2\,\mathrm{dc}\, a\,\mathrm{ns}\, a\, Z(a)-k^2)$$
$$=\int_0^K k^2(\mathrm{sn}(u-a)\,\mathrm{sn}(u+a)-\mathrm{cn}(u-a)\,\mathrm{cn}(u+a))du$$

from those of the Jacobian elliptic functions.[21] The result is

$$\Phi(iu)-\frac{\pi u}{2KK'}i\,\mathrm{cs}\, iu\,\mathrm{dn}\, iu$$
$$=2\left(\frac{\pi}{K'}\right)^2\sum_{n=0}^{\infty}\frac{\cos((2n+1)\pi u/K')}{\sinh^2((2n+1)\pi K/K')}.$$

[21] WW, reference 19, 22.6.

Moreover,[22]

$$iu \operatorname{cs} iu \operatorname{dn} iu - \frac{d}{du}(u \log(-ik^{\frac{1}{2}} \operatorname{sn} iu))$$
$$= -\log(k^{\frac{1}{2}} \operatorname{sc}(u, k')) = \log \cot(\pi u/2K') + \sum_{n=0}^{\infty} \frac{2e^{-(2n+1)\pi K/K'} \cos((2n+1)\pi u/K')}{(2n+1) \sinh((2n+1)\pi K/K')}.$$

Termwise integration of the Fourier series yields the alternative expansion for the partition function

$$-F/NkT = \log \lambda = \tfrac{1}{2} \log(2 \sinh 2H) + \frac{K}{\pi} \int_0^a \Phi(iu)du = y \log(2 \sinh 2H')$$
$$+(\tfrac{1}{2}-y) \log(2 \sinh 2H) + 2\int_0^y \log \cot(\pi z)dz + \frac{1}{\pi} \sum_{n=0}^{\infty} \frac{(1+(4n+2)(\pi i/\tau) - \exp[-(4n+2)\pi i/\tau])}{(2n+1)^2 \sinh^2((2n+1)\pi i/\tau)} \times \sin((4n+2)\pi y). \quad (7.6)$$

The formula (119b) of the text is obtained by specialization to the case $H'=H$; $y=\frac{1}{4}$, with $\tau = 2\tau_1$, whereby

$$\int_0^{\pi/4} \log \cot x \, dx = 1^{-2} - 3^{-2} + 5^{-2} - 7^{-2} + \cdots = G.$$

[22] WW, reference 19, 22.5, example 3.

8. Critical Data

The transition temperature is given by the condition

$$\sinh 2H \sinh 2H' = \sinh(2J/kT) \sinh(2J'/kT) = 1; \quad (T = T_c). \quad (8.1)$$

Then

$$\tau = 0; \quad K = \infty; \quad K' = \tfrac{1}{2}\pi$$
$$\pi y = a = \operatorname{gd} 2H' = \tfrac{1}{2}\pi - \operatorname{gd} 2H. \quad (8.2)$$

The formula (6.1) for the energy becomes

$$U_c = -(2/\pi)(NJ' \operatorname{gd} 2H' \coth 2H' + NJ \operatorname{gd} 2H \coth 2H) \quad (8.3)$$

and the formula (7.6) for the partition function simplifies to

$$-F_c/NkT = \log \lambda_c = \tfrac{1}{2} \log 2 + (\tfrac{1}{2}-2y) \log \cot \pi y + 2\int_0^y \log \cot \pi z \, dz. \quad (8.4)$$

The specific heat becomes infinite; the approximate formula

$$C/Nk \sim (4/\pi)(K(H+H' \sinh 2H)^2 \sinh 2H' - H^2 \sinh^2 2H' \operatorname{gd} 2H - 2HH' - H'^2 \sinh^2 2H \operatorname{gd} 2H') \quad (8.5)$$

where

$$K \sim \log(4/k') \sim \tfrac{1}{2}[\log(4T/|T-T_c|) - \log(H \coth 2H + H' \coth 2H')]$$

is valid for temperatures near the critical point.