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# Antiferromagnetic ordering in the three-state Potts model

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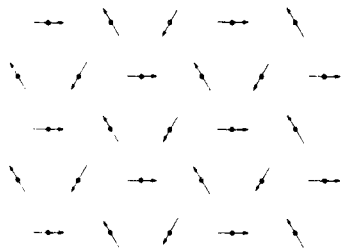
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Received 15 July 1977

**Abstract.** We study the three-state Potts model on a triangular lattice with nearest-neighbour interaction  $K$ . Using a simple position-space renormalisation group transformation we find that, in addition to the usual continuous transition to the ferromagnetic state which occurs for positive  $K$ , a continuous transition to an antiferromagnetic state occurs for negative  $K$ . Our transformation introduces a three-spin interaction. In the space of these two interactions, the lines of ferromagnetic and antiferromagnetic transitions meet at a bicritical point. These results differ from those predicted by Landau theory.

## 1. Introduction

The  $q$ -state Potts model (Potts 1952) with attractive, or ferromagnetic, interactions has been studied extensively. Yet, with the exception of the  $q = 2$  case, the Ising model, little or no attention has been paid to this model with repulsive or antiferromagnetic interactions. Perhaps this is due to the fact that, in general, a repulsive interaction is insufficient to bring about order at any temperature. A case in point is a  $q \geq 3$  system on a square lattice with nearest-neighbour interactions only. However, it is not difficult to conceive of simple Potts systems with repulsive interactions which one would expect to order. For example the 3-state Potts model with nearest-neighbour repulsive interactions should order on a triangular lattice in two dimensions. One of the six possible ground states of the three-state Potts model on the triangular lattice is shown in figure 1. If one includes repulsive interactions between spins at greater distances, more complicated ground states can be stabilised. In the Ising model antiferromagnetic transitions occur which do not belong to the same



**Figure 1.** One of the six possible antiferromagnetic ground states of the three-state Potts model on a triangular lattice.

universality class as the ferromagnetic transition (Domany *et al* 1977, Krinsky and Mukamel 1977). The classes they do belong to, if they are not first order, have been of theoretical interest recently. We expect that the transitions of Potts models with three or more states and antiferromagnetic interactions will likewise belong to different classes than the ferromagnetic transitions unless both are first order. We also hope that these classes will be of interest.

In this paper we examine the three-state Potts model on the triangular lattice. In the following section we present the usual Hamiltonian, extend it to include three-spin interactions and discuss its symmetries. The Landau theory of this system is discussed in § 3 and its prediction of the phase diagram is obtained. In § 4 we carry out a simple position-space renormalisation group calculation and obtain a very different phase diagram. We conclude with a brief summary.

## 2. The Hamiltonian and its symmetries

In order to write the Hamiltonian in a form which is convenient for our purposes we first decompose the triangular lattice into sublattices, *A*, *B*, and *C*, whose lattice constant is  $\sqrt{3}$  larger than that of the original lattice. In figure 1, spins with the same orientation are on the same sublattice. If the nearest-neighbour interaction is denoted *K* then the reduced Hamiltonian can be written as a sum over elementary triangles in the following form:

$$H = -\beta\mathcal{H} = \frac{1}{2}K \sum_i \sum_l (P_{iA}^l P_{iB}^l + P_{iB}^l P_{iC}^l + P_{iA}^l P_{iC}^l) + L \sum_i \sum_l P_{iA}^l P_{iB}^l P_{iC}^l \quad (2.1)$$

where  $\beta = 1/kT$ , the first sum is over all triangles or triples of nearest-neighbour sites, the second sum over the three possible orientations *a*, *b*, and *c* of the Potts spin on each site (see figure 1), and *iA* (*iB*, *iC*) denotes the site of the *i*th triangle which is on sublattice *A* (*B*, *C*). Here  $P_{iA}^l$  is a projection variable which is 1 if the spin on site *iA* has orientation *l*, and 0 otherwise. The usual Potts model is defined with the term *L* in (2.1) equal to zero, but as such a Hamiltonian automatically gives rise to a non-zero *L* in our renormalisation group procedure (§ 4 below), it is convenient to include it explicitly from the start.

The Hamiltonian (2.1) is invariant under all permutations of the spin-orientation labels *a*, *b*, and *c* (carried out simultaneously at all sites of the lattice), which form a group *R*, and also under the translations, rotations, and reflections which comprise the space group *P6mm* of a triangular lattice. As the operations in *R* and *P6mm* commute with each other, the symmetry group *G*<sub>0</sub> of *H* is simply their direct product.

In the special case  $L = -3K/2$ , *H* has an additional symmetry which can be made explicit by defining

$$M \equiv 3K + 2L \quad (2.2)$$

and rewriting (2.1) in the form

$$H = \frac{1}{2}K \sum_i \sum_l (P_{iA}^l P_{iB}^l + P_{iB}^l P_{iC}^l + P_{iA}^l P_{iC}^l - 3P_{iA}^l P_{iB}^l P_{iC}^l) + M \sum_i \sum_l P_{iA}^l P_{iB}^l P_{iC}^l. \quad (2.3)$$

Now define an operation  $\tau$  as follows: it rotates all spins on sublattice *B* clockwise by

$2\pi/3$ , spins on sublattice  $C$  counterclockwise by  $2\pi/3$  and leaves those on  $A$  invariant. That is to say, if  $[lmn]$  denotes the orientations on sublattices  $A, B$ , and  $C$ ,

$$\tau^3[aaa] = \tau^2[abc] = \tau[acb] = [aaa]. \tag{2.4}$$

The term in parentheses in (2.3) is zero for the configurations in (2.4) and those like them (generated from  $(bbb)$  and  $(ccc)$  by the application of  $\tau$ ). Similarly,

$$\tau^3[abb] = \tau^2[aca] = \tau[aac] = [abb], \tag{2.5}$$

and for these configurations and their analogues the term in parentheses in (2.3) is one.

Thus when  $M = 0$ ,  $H$  is invariant under all the transformations generated by products of elements in  $G_0$  and  $\tau$  and  $\tau^2$ . We shall call this larger group  $G_1$ .

### 3. Order parameters and Landau theory

Landau's phenomenological theory predicts that only certain symmetry changes are allowed in second-order or continuous phase transitions, in contrast to first-order transitions (Landau and Lifshitz 1968). We shall show that none of the transitions we are considering are permitted to be second order in the Landau theory, due to the presence of third-order invariants in the appropriate irreducible representations of the symmetry groups.

In applying the Landau theory it is necessary to introduce a set of order parameters, which we shall do as follows. Let us assume that for all values of  $M$  and  $K$  in (2.3), the thermal averages of  $P_{iA}^l, P_{iB}^l$  and  $P_{iC}^l$  are independent of  $i$ , that is, the expectation value for the Potts spin may depend on the sublattices but is identical for all sites on the same sublattice. Introduce the nine quantities

$$n_L^l = \langle P_{iL}^l \rangle \tag{3.1}$$

where  $L = A, B$ , or  $C$  and  $l = a, b$ , or  $c$ . Since  $\sum_i n_L^l$  is equal to 1, only six of the  $n_L^l$  are independent and we introduce the following six independent order parameters (or, equivalently, six components of a vector order parameter):

$$\psi_{1L} = \frac{3}{2}n_L^a - \frac{1}{2} \quad \psi_{2L} = \frac{1}{2}\sqrt{3}(n_L^b - n_L^c). \tag{3.2}$$

One can think of these as the averages of the projections on two orthogonal axes (horizontal and vertical in figure 1) of the Potts spins on sublattice  $L$ . The elements in the group  $R$  permute the labels  $a, b$ , and  $c$ , transforming  $\psi_{1L}$  and  $\psi_{2L}$  ( $L$  fixed) into linear combinations of one another, whereas the operations of the space group  $P6mm$  have the effect of permuting the sublattice labels  $A, B, C$ . The  $\psi_{iL}$  all vanish in the disordered (paramagnetic) state in which every  $n_L^l$  is  $\frac{1}{3}$ .

To discuss ferromagnetic and antiferromagnetic order it is useful to choose the following linear combinations of the  $\psi_{iL}$ :

$$\begin{aligned} \psi_1 &= \sqrt{\frac{1}{3}}(\psi_{1A} + \psi_{1B} + \psi_{1C}) & \psi_2 &= \sqrt{\frac{1}{3}}(\psi_{2A} + \psi_{2B} + \psi_{2C}) \\ \phi_1 &= \sqrt{\frac{2}{3}}(\psi_{1A} - \frac{1}{2}\psi_{1B} - \frac{1}{2}\psi_{1C}) & \phi_2 &= \sqrt{\frac{2}{3}}(\psi_{2A} - \frac{1}{2}\psi_{2B} - \frac{1}{2}\psi_{2C}) \\ \phi_3 &= \sqrt{\frac{1}{2}}(\psi_{1B} - \psi_{1C}) & \phi_4 &= \sqrt{\frac{1}{2}}(\psi_{2B} - \psi_{2C}). \end{aligned} \tag{3.3}$$

In the case of ferromagnetic ordering,  $\psi_{iL}$  is independent of  $L$  (that is, the average direction of the spin is the same on all sublattices), so that the  $\phi_j$  are all zero. In the

case of antiferromagnetic ordering one expects  $\sum_L \psi_{jL}$  to vanish (the 'net magnetisation' is zero) and hence the  $\psi_j$  are both zero. Thus we may call the two-dimensional space spanned by the  $\psi_j$  the 'ferromagnetic' representation  $V_+$  and the four-dimensional space spanned by the  $\phi_j$  the 'antiferromagnetic' representation  $V_-$  of the group  $G_0$ .

Both  $V_+$  and  $V_-$  are irreducible representations of  $G_0$ . In particular  $V_-$  is the Kronecker product of a two-dimensional irreducible representation of  $R$  and a two-dimensional irreducible representation of  $P6mm$ . The latter may be thought of as spanned by the following functions of  $\mathbf{r}$ :  $\sin(\mathbf{k} \cdot \mathbf{r})$  and  $\cos(\mathbf{k} \cdot \mathbf{r})$ , where  $\mathbf{r}$  is the position of a node of the triangular lattice (assuming one node is at the origin), and  $\mathbf{k}$  is a vector in reciprocal space at one of the corners of the first Brillouin zone.

The matrices of the generators of  $G_0$  are given in the appendix. By using them one can confirm that the functions

$$\begin{aligned} f_1 &= \psi_1^3 - 3\psi_1\psi_2^2, \\ f_2 &= \phi_1^3 - 3\phi_1\phi_2^2 - 3\phi_1\phi_3^2 + 3\phi_1\phi_4^2 + 6\phi_2\phi_3\phi_4 \end{aligned} \quad (3.4)$$

on  $V_+$  and  $V_-$ , which are obviously third order and non-vanishing, are invariant under the transformations of  $G_0$ . Hence Landau theory predicts both ferromagnetic to disordered and antiferromagnetic to disordered transitions must be first order, if they occur at all, except, possibly, for special values of the parameters  $K$  and  $M$  where the third-order invariants vanish. The ferromagnetic case has been discussed previously (Straley and Fisher 1973), but not (so far as we know) the antiferromagnetic.

In the case where  $M$  in (2.3) vanishes the Hamiltonian possesses a larger symmetry group  $G_1$ , as noted above in § 2. In this case the sum of the spaces  $V_+ + V_-$  is an irreducible representation of  $G_1$  (see the appendix), and direct calculation shows that the function

$$f_3 = f_1 + f_2/\sqrt{2} \quad (3.5)$$

is an invariant. Thus Landau theory predicts the phase transition from the ordered to disordered state at  $M = 0$  should also be first order (if it occurs).

On the basis of the above considerations one would anticipate a phase diagram in the  $K, M$  plane consisting of three first-order lines separating the disordered and ferromagnetic, the disordered and antiferromagnetic, and the ferromagnetic and antiferromagnetic phases, respectively. The last should lie along a portion of the negative  $K$  axis in the  $K, M$  plane. The phase diagram we obtain using renormalisation group methods (§ 4) has a similar topology, but with the very important difference that the transitions involving the disordered phase are continuous, and a bicritical point occurs instead of a triple point.

#### 4. Renormalisation group approach

In this section we determine the phase diagram of our system using a simple position-space renormalisation group of the type introduced by Niemeier and van Leeuwen (1973, 1974). In order to preserve the antiferromagnetic states under the transformation we must employ at least three cells. Our recursion relations are based on the cluster of three interpenetrating three-spin cells shown in figure 2. Periodic boundary conditions are employed. The same cell and spin assignment has been

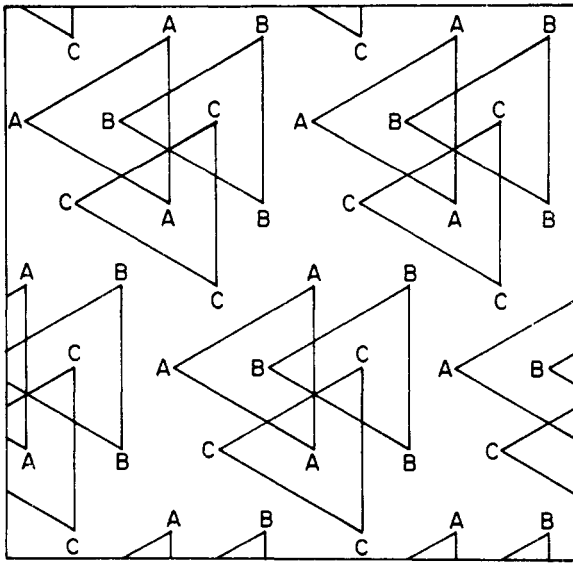


Figure 2. Assignment of site spins to cells.

applied to the Ising antiferromagnet with very good results (Schick *et al* 1976). The configurations of the three site spins within a cell are assigned to one of the three possible cell-spin orientations according to the following prescription. For the twenty-one configurations in which at least two of the site-spin orientations are the same, majority rule is employed. The six configurations of the form  $[abc]$  are each assigned to all three cell-spin states with weight of one third. As noted earlier, our choice of three cells leads to the introduction of a three-spin interaction. The recursion relations are most easily written in terms of  $x = e^{K/2}$  and  $y = e^{M/2}$ . They are

$$x' = [Z(aab)/Z(abc)]^{1/6}, \quad y' = [Z(aaa)/Z(abc)]^{1/6},$$

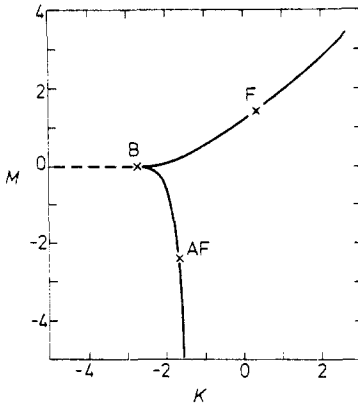
where

$$Z(aaa) = \frac{2}{3}x^{18} + 12x^{15}y + 36x^{14}y^2 + 72x^{13}y^3 + 60x^{12}y^6 + 72x^{12}y^4 + 66x^{12}y^2 + 108x^{11}y^5 + 72x^{11}y^3 + 54x^{10}y^8 + 36x^{10}y^4 + \frac{40}{3}x^9y^3 + 54x^8y^8 + 54x^8y^6 + 18x^6y^{12} + y^{18},$$

$$Z(aab) = \frac{32}{3}x^{18} + 9x^{16}y^2 + 18x^{16} + 30x^{15}y + 45x^{14}y^4 + 42x^{14}y^2 + 111x^{14} + 24x^{13}y^3 + 48x^{13}y + 5x^{12}y^6 + 24x^{12}y^4 + 108x^{12}y^2 + 34x^{12} + 84x^{11}y^3 + 42x^{11}y + 30x^{10}y^4 + 24x^{10}y^2 + 9x^{10} + \frac{94}{3}x^9y^3,$$

$$Z(abc) = \frac{2}{3}x^{18} + 12x^{15}y^2 + 18x^{14}y^2 + 18x^{14} + 72x^{13}y + 102x^{12}y^2 + 96x^{12} + 36x^{11}y^3 + 144x^{11}y + 36x^{10}y^2 + 54x^{10} + \frac{40}{3}x^9y^3 + 81x^8y^2 + 27x^8 + 18x^6 + 1.$$

We find the phase diagram shown in figure 3. The ferromagnetic transition is continuous as is well known (Baxter 1973). The antiferromagnetic transition is also



**Figure 3.** Phase diagram in the space of two- and three-spin interactions. The three critical fixed points are denoted by crosses. The full curves denote continuous transitions and the broken line a first-order transition.

continuous. The two phases meet at a bicritical point. This phase diagram results from seven fixed points. Three of them are uninteresting, being sinks for the three phases. A fourth is simply a discontinuity, or first-order, fixed point located at  $M = 0$ ,  $K \rightarrow -\infty$ . The properties of the three critical fixed points are given in table 1. The ferromagnetic fixed point has one relevant eigenvalue  $Y_1 = 1.04$ . There have been numerous calculations of this eigenvalue. The earliest, by series methods, obtained 1.02 (Straley and Fisher 1973). More recent calculations yield 1.17 from series (Zwanzig and Ramshaw 1977) and 1.20 from variational renormalisation group calculations (Burkhardt *et al* 1976, Dasgupta 1977). The critical temperature of the Hamiltonian with nearest-neighbour interactions only is obtained from the intersection of the critical surface with the line  $M = 3K$ , for along this line the three-spin interaction vanishes (equation (2.2)). This intersection yields  $K_c(F) = 0.53$ . The exact value is 0.63 (Kim and Joseph 1974). The antiferromagnetic fixed point has one relevant eigenvalue  $Y_1 = 1.11$ . With nearest-neighbour interactions only the critical coupling is  $K_c(AF) = -1.56$ . Finally the eigenvalues of the bicritical point are both relevant, being 1.99 and 0.87. The phase diagram obtained here differs greatly from that predicted by mean-field theory. The sole agreement between them is the obvious coexistence of the ferromagnetic and antiferromagnetic phases at low temperatures along the line  $M = 0$ .

**Table 1.** Properties of critical fixed points.

Designation	Name	Location	Eigenvalues
F	ferromagnetic	$K^* = 0.32$ $M^* = 1.44$	$Y_1 = 1.04$ $Y_2 = -1.79$
AF	antiferromagnetic	$K^* = -1.68$ $M^* = -2.39$	$Y_1 = 1.11$ $Y_2 = -1.90$
B	bicritical	$K^* = -2.72$ $M^* = 0$	$Y_1 = 1.99$ $Y_2 = 0.87$

### 5. Conclusions

The renormalisation group calculation carried out above confirms our expectation that Potts systems can undergo antiferromagnetic transitions. On a two-dimensional triangular lattice the antiferromagnetic transition is continuous and belongs to a different universality class from the ferromagnetic transition. This is consistent with the fact that the order parameter for the former was found to have four components while that of the latter has only two. The transition on the line  $M = 0$ , corresponding to the bicritical point in the phase diagram in figure 3, has properties distinct from either the ferromagnetic or antiferromagnetic transitions. This is again consistent with the fact that the order parameter was found to have six components. Aside from the ferromagnetic case, these classes of transitions have not, to our knowledge, been studied previously.

### Acknowledgments

MS would particularly like to thank Eytan Domany for several stimulating and encouraging conversations. He has also profited from discussions with M E Fisher, G R Golner, E K Riedel, and J S Walker. RBG would like to express appreciation for the hospitality of the Department of Physics of the University of Washington. Support of the National Science Foundation under grant numbers DMR-73-02582 A02 and DMR-76-23071 is gratefully acknowledged.

### Appendix. Representations of $G_0$ and $G_1$

The transformations of  $V_+$  and  $V_-$  (§ 3) under  $R$  and  $P6mm$  can be obtained as follows. The group  $R$  consists of permutations of the labels of three Potts states  $a$ ,  $b$ , and  $c$ . If we denote the permutations of  $a$  with  $b$  by the normal notation  $(ab)$ , etc, then we can write

$$(ab)n_L^a = n_L^b \tag{A.1}$$

etc. Using the fact that  $\sum_i n_L^i = 1$ , one can show that

$$\begin{aligned} (ab)\psi_{1L} &= \frac{1}{2}\sqrt{3}\psi_{2L} - \frac{1}{2}\psi_{1L} \\ (ab)\psi_{2L} &= \frac{1}{2}\sqrt{3}\psi_{1L} + \frac{1}{2}\psi_{2L} \\ (bc)\psi_{1L} &= \psi_{1L}; \quad (bc)\psi_{2L} = -\psi_{2L} \end{aligned} \tag{A.2}$$

and hence

$$\begin{aligned} (ab)\psi_1 &= \frac{1}{2}\sqrt{3}\psi_2 - \frac{1}{2}\psi_1 & (bc)\psi_1 &= \psi_1 \\ (ab)\psi_2 &= \frac{1}{2}\sqrt{3}\psi_1 + \frac{1}{2}\psi_2 & (bc)\psi_2 &= -\psi_2 \\ (ab)\phi_1 &= -\frac{1}{2}\phi_1 + \frac{1}{2}\sqrt{3}\phi_2 & (bc)\phi_1 &= \phi_1 \\ (ab)\phi_2 &= \frac{1}{2}\sqrt{3}\phi_1 + \frac{1}{2}\phi_2 & (bc)\phi_2 &= -\phi_2 \\ (ab)\phi_3 &= -\frac{1}{2}\phi_3 + \frac{1}{2}\sqrt{3}\phi_4 & (bc)\phi_3 &= \phi_3 \\ (ab)\phi_4 &= \frac{1}{2}\sqrt{3}\phi_3 + \frac{1}{2}\phi_4 & (bc)\phi_4 &= -\phi_4. \end{aligned} \tag{A.3}$$



The operations of  $P6mm$  do not alter the spin orientations, but have the effect of interchanging the sublattices. It is obvious that any permutation of the sublattices can be obtained by some operation in  $P6mm$ , and hence the transformations on  $V_+$  and  $V_-$  are conveniently designated by (AB), for the interchange of sublattices A and B, etc. Thus one has

$$\begin{aligned}
 (AB)\psi_1 &= (BC)\psi_1 = \psi_1 & (AB)\psi_2 &= (BC)\psi_2 = \psi_2 \\
 (AB)\phi_1 &= -\frac{1}{2}\phi_1 + \frac{1}{2}\sqrt{3}\phi_3 & (BC)\phi_1 &= \phi_1 \\
 (AB)\phi_2 &= -\frac{1}{2}\phi_2 + \frac{1}{2}\sqrt{3}\phi_4 & (BC)\phi_2 &= \phi_2 \\
 (AB)\phi_3 &= \frac{1}{2}\sqrt{3}\phi_1 + \frac{1}{2}\phi_3 & (BC)\phi_3 &= -\phi_3 \\
 (AB)\phi_4 &= \frac{1}{2}\sqrt{3}\phi_2 + \frac{1}{2}\phi_4 & (BC)\phi_4 &= -\phi_4.
 \end{aligned} \tag{A.4}$$

The other transformations of  $G_0$  and  $V_+$  and  $V_-$  can be obtained by using products of the generators ( $ab$ ), ( $bc$ ), (AB), and (BC). One can verify directly that the functions  $f_1$  and  $f_2$  in (3.4) are invariant under these generators, and hence they are also invariant under  $G_0$ .

The transformations of  $\tau$  on  $V = V_+ + V_-$  can be obtained in a straightforward way using the definition in § 2; i.e.  $\tau$  is the permutation,  $a$  goes to  $b$  goes to  $c$  goes to  $a$ , denoted ( $abc$ ), when  $L = B$ , and ( $acb$ ) when  $L = C$ . The result is:

$$\begin{aligned}
 \tau\psi_1 &= \sqrt{\frac{1}{2}}\phi_1 + \sqrt{\frac{1}{2}}\phi_4 \\
 \tau\psi_2 &= \sqrt{\frac{1}{2}}\phi_2 - \sqrt{\frac{1}{2}}\phi_3 \\
 \tau\phi_1 &= \sqrt{\frac{1}{2}}\psi_1 + \frac{1}{2}\phi_1 - \frac{1}{2}\phi_4 \\
 \tau\phi_2 &= \sqrt{\frac{1}{2}}\psi_2 + \frac{1}{2}\phi_2 + \frac{1}{2}\phi_3 \\
 \tau\phi_3 &= \sqrt{\frac{1}{2}}\psi_2 - \frac{1}{2}\phi_2 - \frac{1}{2}\phi_3 \\
 \tau\phi_4 &= -\sqrt{\frac{1}{2}}\psi_1 + \frac{1}{2}\phi_1 - \frac{1}{2}\phi_4.
 \end{aligned} \tag{A.5}$$

The group  $G_1$  is generated from  $\tau$  and  $G_0$ , and hence its transformations on  $V$  can be obtained by successive applications of the five generators ( $ab$ ), ( $bc$ ), (AB), (BC), and  $\tau$ . One can show that  $V$  is an irreducible representation of  $G_1$  in the following manner. Evidently  $V_+$  and  $V_-$  are inequivalent irreducible representations of  $G_0$ , and hence, by Schur's lemmas (Hamermesh 1962), any transformation  $Q$  which commutes with all the transformations of  $G_0$  has the form  $\mu 1_+ + \lambda 1_-$  where  $1_+$  is the identity (unit matrix) on  $V_+$ ,  $1_-$  the identity on  $V_-$ , and  $\mu$  and  $\lambda$  are real numbers. However, such a transformation commutes with  $\tau$ —see (A.5) above—only if  $\lambda = \mu$ . As the transformations of  $G_1$  on  $V$  include all those of  $G_0$  and also  $\tau$ , we see that only a multiple of the identity will commute with all the matrices of  $G_1$ , and thus  $V$  forms an irreducible representation of  $G_1$ .

The function  $f_3$  in (3.5) is, evidently, invariant under all the transformations of  $G_0$ . Thus its invariance under  $G_1$  follows from the fact (which can be checked by a direct calculation) that it is invariant under  $\tau$ .

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