

Theory of the phase transition of He³ into the superfluid state

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We find all 18 Landau energy extrema for the phase transition of He³ into the superfluid state.

It is well known that the transition of He³ into the superfluid state is described satisfactorily in the framework of Landau's general second-order phase transition theory. The superfluidity of He³ is caused by the Bose-Einstein condensation of Cooper pairs with spin $S = 1$ and angular momentum $L = 1$. The order parameter is therefore a ψ -function which has spin (Greek) and orbital (Roman) vector indexes $\psi_{i\alpha}$. If one neglects the dipole-dipole interaction of the nuclear spins, the Landau energy is equal to

$$F = -\tau \psi_{i\alpha} \psi_{i\alpha}^* + 1/2 \{ \beta_1 \psi_{i\alpha} \psi_{i\alpha} \psi_{j\beta}^* \psi_{j\beta}^* + \beta_2 (\psi_{i\alpha} \psi_{i\alpha}^*)^2 + \beta_3 \psi_{i\alpha} \psi_{j\beta}^* \psi_{j\alpha} \psi_{i\beta}^* + \beta_4 \psi_{i\alpha} \psi_{j\beta}^* \psi_{j\alpha} \psi_{i\beta}^* + \beta_5 \psi_{i\alpha} \psi_{j\beta}^* \psi_{j\alpha} \psi_{i\beta}^* \} \quad (1)$$

(see Refs. 1,2). The equilibrium equations

$$\delta F / \delta \psi_{i\alpha} = 0 \quad (2)$$

have solutions with a continuous degeneracy with respect to rotations of the spin and orbital spaces and to gauge transformations. As a consequence of this there are difficulties of analytically solving the equations. Three solutions, corresponding to the A -, and B -phases of He³ and to the planar phase have been known from the microscopic theory.³⁻⁵ Another three were found analytically in Refs. 1, 2, 6. Barton and Moore⁷ analyzing the problem numerically found six new solutions. Finally, Jones⁸ discovered a thirteenth, very complicated solution. Although there can no longer be any doubts about the structure of the superfluid phases of He³ it would nonetheless be desirable to know all extrema of the energy (1).

1. We introduce new variables φ_{ij} and f_{ij} :

$$\varphi_{ij} = \psi_{i\alpha} \psi_{j\alpha}, \quad f_{ij} = \psi_{i\alpha} \psi_{j\alpha}^* \quad (3)$$

In those variables the energy is equal to

$$F = -\tau f + 1/2 \{ \beta_1 \varphi \varphi^* + \beta_2 f^2 + \beta_3 \varphi_{ij} \varphi_{ij}^* + \beta_4 f_{ij} f_{ji} + \beta_5 f_{ij} f_{ij} \}, \quad (4)$$

where $f = f_{ii}$, $\varphi = \varphi_{ii}$. Multiplying Eq. (2) by $\psi_{j\alpha}^*$ and summing over the spin index we get

$$\psi_{j\alpha}^* \delta F / \delta \psi_{i\alpha} = -\tau f_{ij} + \beta_1 \varphi \varphi_{ij}^* + \beta_2 f f_{ij} + \beta_3 \varphi_{ik} \varphi_{kj}^* + \beta_4 f_{ik} f_{kj} + \beta_5 f_{ik} f_{kj} = 0. \quad (5)$$

Repeating this procedure with the function $\psi_{j\alpha}$ we get

$$\psi_{j\alpha} \delta F / \delta \psi_{i\alpha}^* = -\tau \varphi_{ij} + \beta_1 \varphi_{ij} \varphi + \beta_2 f \varphi_{ij} + \beta_3 \varphi_{ik} \varphi_{kj} + \beta_4 f_{ik} \varphi_{kj} + \beta_5 f_{ik} \varphi_{kj} = 0. \quad (6)$$

Evaluating the trace of Eq. (5) with respect of the orbital index $\psi_{i\alpha}^* \delta F / \delta \psi_{i\alpha}^* = 0$, we can check that for the solutions of Eqs. (5), (6) the energy (4) is equal to

$$F = -\tau f / 2. \quad (7)$$

We separate the real and imaginary parts of the symmetric matrix φ_{ij}

$$\varphi_{ij} = A_{ij} + i B_{ij}. \quad (8)$$

Using the freedom of choice of the phase of the ψ -function, we put $B_{ii} = 0$. The real part χ_{ij} of the matrix f_{ij} is symmetric and the imaginary part antisymmetric. Introducing an appropriate dual vector b_k we have

$$f_{ij} = \chi_{ij} + i e_{ijk} b_k. \quad (9)$$

We separate in Eqs. (5) and (6) the real and imaginary, and the symmetric and anti-symmetric parts:¹¹

$$\begin{aligned} \text{I } & (\beta_2 \chi - \tau) \chi_{ij} + \beta_1 A_{ij} + \beta_3 (A_{ik} A_{kj} + B_{ik} B_{kj}) + (\beta_4 + \beta_5) \chi_{ik} \chi_{kj} = (\beta_4 - \beta_5) (b_i b_j - \delta_{ij} b^2), \\ \text{II } & \beta_1 A B_{ij} = \beta_5 (\chi_{ik} e_{kjn} + \chi_{kj} e_{kin}) b_n, \\ \text{III } & (\beta_2 \chi - \tau) A_{ij} + \beta_1 A_{ij} + \gamma (\chi_{ik} A_{kj} + \chi_{jk} A_{ki}) = \mu (e_{ikn} B_{nj} + e_{jkn} B_{ki}) b_n, \\ \text{IV } & (\beta_2 \chi - \tau) B_{ij} + \gamma (\chi_{ik} B_{kj} + \chi_{jk} B_{ki}) = \mu (e_{ikn} A_{kj} + e_{jkn} A_{ki}) b_n, \\ \text{V } & (\beta_2 \chi - \tau) b_n + \beta_3 e_{ijn} B_{ik} A_{kj} = \beta_4 (\chi_{ni} b_i - \chi b_n), \\ \text{VI } & v e_{ijn} \chi_{ik} A_{kj} + \eta b_j B_{jn} = 0, \\ \text{VII } & \beta_1 A b_n + v e_{ijn} \chi_{jk} B_{ki} = \eta (b_n A - b_j A_{nj}). \end{aligned} \quad (10)$$

Here $\chi = \chi_{ii}$, $A = A_{ii}$, $b^2 = b_i b_i$, $\gamma = (\beta_3 + \beta_4 + \beta_5)/2$, $\mu = (\beta_3 + \beta_4 - \beta_5)/2$, $v = (\beta_4 + \beta_5 - \beta_3)/2$, $\eta = (\beta_4 - \beta_5 - \beta_3)/2$. We choose Cartesian coordinates in the orbital x, y, z -space such that the matrix χ_{ij} is diagonal. Thus, changing to new variables A_{ij} , B_{ij} , χ_{ij} , b_i we are completely rid of the continuous degeneracy. The price of this simplification are redundant solutions which may appear in connection with the multiplication when we changed from (2) to (5) and (6). In fact, one can easily identify the redundant solutions thanks to the following fact. One can perform a similar transformation to introduce a set of equations for the traces with respect to the orbital indexes $\psi_{i\alpha} \psi_{i\beta}$, $\psi_{i\alpha} \psi_{i\beta}^*$. The corresponding set of equations then differs from (5) and (6) only through the substitution $\beta_3 \rightleftharpoons \beta_5$. It is thus clear that those solutions of the set (10) which do not have a partner with an energy differing through the substitution $\beta_3 \rightleftharpoons \beta_5$ must be dropped.

Bearing this selection rule in mind we first find all possible values of the quantity χ . This can be done even without a complete analysis of all equations of the set (10). After dropping the clearly redundant values of χ there remain 18 solutions. Of them 13 correspond to earlier known extrema; we shall analyze the other 5 in more detail—we shall see that all of them are extrema of the energy (1).

Let $A \neq 0$; it then follows from (10.II) that $B_{xx} = B_{yy} = B_{zz} = 0$ and

$$\begin{aligned} B_{xy} &= \frac{\beta_5 b_z}{\beta_1 A} (\chi_{xx} - \chi_{yy}), \quad B_{yz} = \frac{\beta_5 b_x}{\beta_1 A} (\chi_{yy} - \chi_{zz}), \\ B_{zx} &= \frac{\beta_5 b_y}{\beta_1 A} (\chi_{zz} - \chi_{xx}). \end{aligned} \quad (11)$$

Substituting these values of the B_{ik} components into (10.VI) we find

$$\begin{aligned} (\chi_{xx}-\chi_{yy})(\nu A_{xy}-\eta\beta_3 b_x b_y/\beta_1 A) &= 0, \\ (\chi_{yy}-\chi_{zz})(\nu A_{yz}-\eta\beta_3 b_y b_z/\beta_1 A) &= 0, \\ (\chi_{zz}-\chi_{xx})(\nu A_{zx}-\eta\beta_3 b_z b_x/\beta_1 A) &= 0. \end{aligned} \quad (12)$$

Hence follow three cases:

$$\begin{aligned} 1) \chi_{xx} &= \chi_{yy} = \chi_{zz}, \\ 2) \chi_{xx} &= \chi_{yy}, \quad A_{yz} = \frac{\eta\beta_3}{\nu\beta_1 A} b_y b_z, \quad A_{zx} = \frac{\eta\beta_3}{\nu\beta_1 A} b_x b_z, \\ 3) \chi_{xx} &\neq \chi_{yy} \neq \chi_{zz} \neq \chi_{xx}, \end{aligned} \quad (13)$$

$$A_{ij} = \frac{\eta\beta_3}{\nu\beta_1 A} b_i b_j, \quad i \neq j.$$

Using the free rotation in the orbital space ($b_x = b_y = 0$ we choose in case 1), and for $b_z \neq 0$ we obtain $A_{xy} = 0$ through a rotation around the z -axis. From the x, y components of Eq. (10.VII) we see also that $A_{xz} = A_{yz} = 0$. When $b_z = 0$ we can diagonalize the A_{ik} matrix. In case 2), using the free rotation around the z -axis, we put $b_y = 0$. Then, if $b_x \neq 0$, it follows from the y -component of Eq. (10) that $A_{xy} = 0$; if, however, $b_x = 0$, we can achieve $A_{xy} = 0$ through rotation around the z -axis. Thus, we may assume that Eqs. (13) are correct both in case 1) and in case 2) and we can therefore consider them simultaneously with case 3). Substituting Eqs. (11) and (13) into Eqs. (10.III) (for $i \neq j$) we find

$$\begin{aligned} b_x b_y \{ \beta_2 \chi - \tau + \gamma (\chi - \chi_{zz}) - \mu\nu (3\chi_{zz} - \chi) / \eta \} &= 0, \\ b_y b_z \{ \beta_2 \chi - \tau + \gamma (\chi - \chi_{xx}) - \mu\nu (3\chi_{xx} - \chi) / \eta \} &= 0, \\ b_x b_z \{ \beta_2 \chi - \tau + \gamma (\chi - \chi_{yy}) - \mu\nu (3\chi_{yy} - \chi) / \eta \} &= 0. \end{aligned}$$

Hence we have two possibilities: either $b_x = b_y = 0$, or $b_z = 0$; $b_x, b_y \neq 0$ and

$$\beta_2 \chi - \tau + \gamma (\chi - \chi_{zz}) - \mu\nu (3\chi_{zz} - \chi) / \eta = 0. \quad (14)$$

We show that in the latter case the set of Eqs. (10) is incompatible. To do that it is sufficient to consider only the following 8 equations of the set (10): I— xy -component; III— xx, yy, zz ; V— x, y ; VII— x, y . Using Eqs. (11), (13) we have when $b_z = 0$; $b_x, b_y \neq 0$

$$\begin{aligned} \text{I} \quad \frac{\eta}{\nu} \beta_5 + \beta_5 - \beta_4 + \beta_3 \left[(A - A_{zz}) \frac{\eta\beta_5}{\nu\beta_1 A} + \frac{\beta_5^2}{\beta_1^2 A^2} (\chi_{yy} - \chi_{zz}) (\chi_{zz} - \chi_{xx}) \right] &= 0, \\ \text{II} \quad (\beta_2 \chi - \tau + 2\gamma \chi_{xx}) A_{xx} + \beta_1 A \chi_{xx} &= \frac{2\mu\beta_5}{\beta_1 A} b_y^2 (\chi_{zz} - \chi_{xx}), \\ \text{III} \quad (\beta_2 \chi - \tau + 2\gamma \chi_{yy}) A_{yy} + \beta_1 A \chi_{yy} &= \frac{2\mu\beta_5}{\beta_1 A} b_x^2 (\chi_{zz} - \chi_{yy}), \\ \text{IV} \quad (\beta_2 \chi - \tau + 2\gamma \chi_{zz}) A_{zz} + \beta_1 A \chi_{zz} &= \frac{2\mu b_5}{\beta_1 A} [b_x^2 (\chi_{yy} - \chi_{zz}) - b_y^2 (\chi_{zz} - \chi_{xx})], \\ \text{V} \quad \beta_2 \chi - \tau + \beta_4 (\chi_{yy} + \chi_{zz}) + \frac{\beta_3 \beta_5}{\beta_1 A} (A_{zz} - A_{yy}) (\chi_{yy} - \chi_{zz}) &= \frac{\eta\beta_5 \beta_5^2}{\nu\beta_1^2 A^2} b_y^2 (\chi_{zz} - \chi_{xx}), \\ \text{VI} \quad \beta_2 \chi - \tau + \beta_4 (\chi_{xx} + \chi_{zz}) + \frac{\beta_3 \beta_5}{\beta_1 A} (A_{zz} - A_{yy}) (\chi_{yy} - \chi_{zz}) &= \frac{\eta\beta_5 \beta_5^2}{\nu\beta_1^2 A^2} b_x^2 (\chi_{zz} - \chi_{yy}), \end{aligned}$$

$$= \frac{\eta\beta_5 \beta_5^2}{\nu\beta_1^2 A^2} b_y^2 (\chi_{zz} - \chi_{yy}),$$

$$\text{VII} \quad \beta_1 A - \frac{\nu\beta_5}{\beta_1 A} (\chi_{yy} - \chi_{zz})^2 + \eta (A_{xx} - A) + \frac{\eta^2 \beta_5}{\nu\beta_1 A} b_y^2 = 0,$$

$$\text{VIII} \quad \beta_1 A - \frac{\nu\beta_5}{\beta_1 A} (\chi_{xx} - \chi_{zz})^2 + \eta (A_{yy} - A) + \frac{\eta^2 \beta_5}{\nu\beta_1 A} b_x^2 = 0. \quad (15)$$

Adding Eqs. II, III, IV of the set (15) we get

$$(\beta_2 \chi - \tau + \beta_1 \chi) A + 2\gamma (\chi_{xx} A_{xx} + \chi_{yy} A_{yy} + \chi_{zz} A_{zz}) = 0. \quad (16)$$

Using (15.V, VI) we eliminate b_x, b_y from (15.IV), and using (16) we reduce (15.IV) to the form

$$\begin{aligned} \frac{A_{zz}}{A} \frac{\beta_3 \beta_5}{\beta_1} \left\{ \chi - 3\chi_{zz} + \frac{\eta}{2\mu\nu} (\beta_2 \chi - \tau + 2\gamma \chi_{zz}) \right\} + 2(\beta_2 \chi - \tau) \\ + \beta_4 (\chi + \chi_{zz}) + \frac{\beta_3 \beta_5}{2\beta_1 \gamma} (\beta_2 \chi - \tau + \beta_1 \chi + 2\gamma \chi_{zz}) + \frac{\beta_3 \beta_5}{2\mu\nu} \chi_{zz} = 0. \end{aligned} \quad (17)$$

We now use (15.VII, VIII) to eliminate b_x, b_y from Eq. (15.IV). Using (16) and (15.I) we get

$$\begin{aligned} -\eta \frac{A_{zz}}{A} \left\{ \chi - 3\chi_{zz} + \frac{\eta}{2\mu\nu} (\beta_2 \chi - \tau + 2\gamma \chi_{zz}) \right\} + \beta_1 (3\chi_{zz} - \chi) \\ + \eta (2\chi - 5\chi_{zz}) + \frac{\beta_1}{\beta_3 \beta_5} (\eta\beta_5 + \nu\beta_5 - \nu\beta_4) (\chi - 3\chi_{zz}) \\ + \frac{\eta}{2\gamma} (\beta_2 \chi - \tau + \beta_1 \chi) - \frac{\beta_1 \eta^2}{2\mu\nu} \chi_{zz} = 0. \end{aligned} \quad (18)$$

We have thus three Eqs. (14), (17), (18) for three unknowns $\chi, \chi_{zz}, A_{zz}/A$. One easily checks that this set has a unique solution. It turns out, however, that one can find the ratio A_{zz}/A independently. Indeed, we use (15.VII, VIII) to eliminate b_x, b_y from (15.V, VI) and we find the difference of the equations obtained

$$(\chi_{yy} - \chi_{xx}) \left\{ \beta_1 - \eta + \frac{\beta_1 \eta \beta_4}{\beta_3 \beta_5} - \frac{\nu\beta_5}{\beta_1 A} (\chi_{zz} - \chi_{yy}) (\chi_{zz} - \chi_{xx}) \right\} = 0,$$

whence, since $\chi_{xx} \neq \chi_{yy}$ (otherwise we could assume that $b_y = 0$) we find easily by using (15.I),

$$\frac{A_{zz}}{A} = -\frac{\beta_1}{\eta\beta_3\beta_5} \{ (\beta_4 - \beta_5) (\beta_4 - \beta_5) + \beta_3 \beta_5 \},$$

which contradicts the set of Eqs. (14), (17), (18).

Let now $b_x = b_y = 0, b_z \neq 0$. The zz -components of Eqs. (10.I, II) then have the form

$$\begin{aligned} (\beta_2 \chi - \tau) \chi_{zz} + \beta_1 A A_{zz} + \beta_3 A_{zz}^2 + (\beta_4 + \beta_5) \chi_{zz} &= 0, \\ (\beta_2 \chi - \tau) A_{zz} + \beta_1 A \chi_{zz} + 2\gamma \chi_{zz} A_{zz} &= 0. \end{aligned}$$

Adding and subtracting these equations we get

$$(\chi_{zz} \pm A_{zz}) \{ \beta_2 \chi - \tau + (\beta_4 + \beta_5) \chi_{zz} \pm (\beta_1 A + \beta_3 A_{zz}) \}, \quad (19)$$

whence we have three cases:

$$\begin{aligned} 1) \chi_{zz} &= A_{zz} = 0, \\ 2) \beta_2 \chi - \tau + (\beta_4 + \beta_5) \chi_{zz} &= 0, \quad \beta_1 A + \beta_3 A_{zz} = 0, \\ 3) A_{zz} &= \chi_{zz}, \quad \beta_2 \chi - \tau + (\beta_4 + \beta_5) \chi_{zz} + \beta_1 A + \beta_3 A_{zz} = 0 \end{aligned} \quad (20)$$

(we note here that the case $A_{zz} = -\chi_{zz}$ differs from 3) only through the substitution $\psi \rightarrow i\psi$). When $b_z \neq 0$ the xy -component of Eq. (10.IV) and the z -component of Eqs.

(10.V, VII) reduce to the following relations:

$$\begin{aligned} \frac{\beta_5}{\beta_1 A} \{ \beta_2 \chi - \tau + \gamma (\chi - \chi_{zz}) \} (\chi_{xx} - \chi_{yy}) &= \mu (A_{xx} - A_{yy}), \\ \beta_2 \chi - \tau + \beta_4 (\chi - \chi_{zz}) &= \frac{\beta_2 \beta_5}{\beta_1 A} (A_{xx} - A_{yy}) (\chi_{xx} - \chi_{yy}), \\ \beta_1 A - \eta (A - A_{zz}) &= \frac{\nu \beta_5}{\beta_1 A} (\chi_{xx} - \chi_{yy})^2. \end{aligned}$$

Eliminating from these $A_{xx} - A_{yy}$ and $\chi_{xx} - \chi_{yy}$ we find

$$\begin{aligned} \beta_2 \chi - \tau + \beta_4 (\chi - \chi_{zz}) \\ = \frac{\beta_2 \beta_5}{\mu \nu} \{ \beta_2 \chi - \tau + \gamma (\chi - \chi_{zz}) \} \left\{ 1 - \frac{\eta}{\beta_1} \left(1 - \frac{A_{zz}}{A} \right) \right\} = 0. \end{aligned} \quad (21)$$

In case 1) of Eqs. (20) we get from Eq. (21)

$$\frac{\tau}{\chi} = \beta_2 + \frac{\beta_1 \{ \beta_4 (\beta_3 + \beta_4 + \beta_5) + 2\beta_3 \beta_5 \} + \beta_3 \beta_5 (\beta_3 + \beta_4 + \beta_5)}{\beta_1 (\beta_3 + \beta_4 + \beta_5) + 2\beta_3 \beta_5},$$

which corresponds to the solution found by Jones.⁸ Following Ref. 7 we shall call this solution the η -phase.

In case 2) of (20) we find by using 2) of (20) to eliminate χ_{zz} and A_{zz}/A from (21)

$$\begin{aligned} \frac{\tau}{\chi} = \beta_2 + \left\{ \beta_4 - \frac{\beta_2 \beta_5}{\mu \nu} \gamma \left(1 - \frac{\eta}{\beta_1} - \frac{\eta}{\beta_3} \right) \right\} \\ \times \left\{ 1 + \frac{\beta_4}{\beta_4 + \beta_5} - \frac{\beta_2 \beta_5}{\mu \nu} \left(1 + \frac{\gamma}{\beta_4 + \beta_5} \right) \left(1 - \frac{\eta}{\beta_1} - \frac{\eta}{\beta_3} \right) \right\}^{-1}. \end{aligned}$$

Here and in what follows we indicate values of χ which do not satisfy the above selection criteria by an (*) sign.

Case 3) of (20) can most simply be considered as follows. We introduce real spin vectors \mathbf{l}_i and \mathbf{m}_i such that

$$\{ \psi_{i\alpha} \} = \psi_i = \mathbf{l}_i + i \mathbf{m}_i.$$

Then

$$\chi_{zz} = \mathbf{l}_z^2 + \mathbf{m}_z^2, \quad A_{zz} = \mathbf{l}_z^2 - \mathbf{m}_z^2$$

and from the condition $\chi_{zz} = A_{zz}$ we have $m_z = 0$. The remaining conditions lead to the following relations

$$\begin{aligned} B_{xx} = 2\mathbf{l}_x \mathbf{m}_x = 0, \quad B_{yy} = 2\mathbf{l}_y \mathbf{m}_y = 0, \\ B_{yz} = \mathbf{l}_y \mathbf{m}_z = 0, \quad B_{zx} = \mathbf{l}_z \mathbf{m}_x = 0, \quad A_{xx} = \mathbf{l}_x^2 = 0, \quad A_{yy} = \mathbf{l}_y^2 = 0, \\ \chi_{xy} = \mathbf{l}_x \mathbf{l}_y + \mathbf{m}_x \mathbf{m}_y = 0, \quad A_{xy} = \mathbf{l}_x \mathbf{l}_y - \mathbf{m}_x \mathbf{m}_y = 0, \end{aligned}$$

whence follows that $\mathbf{l}_z \perp \mathbf{l}_x \perp \mathbf{l}_y$ and $\mathbf{m}_x \parallel \mathbf{l}_y$, $\mathbf{m}_y \parallel \mathbf{l}_x$. As a result we can write the $\psi_{i\alpha}$ matrix in the form

$$\chi^{1/2} \begin{pmatrix} \sin \omega \sin \alpha \sin \rho & -i \sin \omega \cos \alpha \sin \zeta & 0 \\ i \sin \omega \cos \alpha \cos \zeta & \sin \omega \sin \alpha \cos \rho & 0 \\ 0 & 0 & \cos \omega \end{pmatrix}. \quad (22)$$

$$\frac{\tau}{\chi} = \beta_2 + \frac{\beta_1^2 \gamma (\beta_4^2 - 4\beta_4 \gamma - 4\beta_3 \beta_5) + \beta_1 \beta_3 \beta_5 (8\gamma^2 + 6\beta_4 \gamma + 12\beta_3 \beta_5) + 8\beta_3^2 \beta_5^2 \gamma}{2(\beta_1 \gamma + \beta_3 \beta_5) \{ \beta_1 (2\beta_4 \gamma + 4\beta_3 \beta_5 \pm \gamma D) + 6\gamma \beta_3 \beta_5 \}}. \quad (27)$$

The solutions (27) which we have found differ one from the other only quantitatively; we call them the Θ^+ - and Θ^- -phases.

When $b_z = 0$ it follows from the condition $\chi_{ik} = A_{ik} = 0$ ($i \neq k$), $B_{ik} = 0$, $b_i = 0$ that all spin vectors \mathbf{l}_i and \mathbf{m}_i are mutually perpendicular so that there cannot be more than three of them. As a result three forms of the $\psi_{i\alpha}$ matrix are possible

$$\begin{pmatrix} \sin \theta \sin \varphi & 0 & 0 \\ 0 & \sin \theta \cos \varphi & 0 \\ 0 & 0 & \cos \theta \end{pmatrix}, \begin{pmatrix} \sin \theta \sin \varphi & 0 & 0 \\ 0 & \sin \theta \cos \varphi & 0 \\ 0 & 0 & i \cos \theta \end{pmatrix}, \begin{pmatrix} \cos \theta & 0 & 0 \\ 0 & \sin \theta \sin \varphi & i \sin \theta \cos \varphi \\ 0 & 0 & 0 \end{pmatrix} \quad (28)$$

The part of the energy (1) which depends on the angles ω , α , ρ , ζ is equal to

$$\begin{aligned} \beta_1 (\cos^2 \omega - \sin^2 \omega \cos 2\alpha)^2 + \frac{\beta_4}{2} \sin^4 \omega \sin^2 2\alpha + 2\gamma \cos^4 \omega \\ + \gamma \sin^4 \omega (\sin^4 \alpha + \cos^4 \alpha + \sin^4 \alpha \cos^2 2\rho + \cos^4 \alpha \cos^2 2\zeta) \\ + \frac{\eta}{2} \sin^4 \omega \sin^2 2\alpha \sin 2\rho \sin 2\zeta \\ + \frac{\beta_5 - \beta_3}{2} \sin^4 \omega \sin^2 2\alpha \cos 2\rho \cos 2\zeta. \end{aligned} \quad (23)$$

The extrema of expression (23) with respect to the angles ρ , ζ correspond either to $\sin 2\rho = \sin 2\zeta = 0$ and then we get for $b_z \neq 0$ the axially symmetric phase of Ref. 7 or to $\cos 2\rho = \cos 2\zeta = 0$ and then we get the ζ -phase of Ref. 7;²⁾ or, finally,

$$\begin{aligned} \frac{\eta}{\gamma} \operatorname{ctg}^2 \alpha \frac{\sin 2\zeta}{\sin 2\rho} + \frac{\beta_5 - \beta_3}{\gamma} \operatorname{ctg}^2 \alpha \frac{\cos 2\zeta}{\cos 2\rho} = 1, \\ \frac{\eta}{\gamma} \operatorname{tg}^2 \alpha \frac{\sin 2\rho}{\sin 2\zeta} + \frac{\beta_5 - \beta_3}{\gamma} \operatorname{tg}^2 \alpha \frac{\cos 2\rho}{\cos 2\zeta} = 1, \end{aligned}$$

whence we find

$$\begin{aligned} \cos 2\rho = \pm \left(\frac{\operatorname{ctg}^2 \alpha - x^2}{y^2 - x^2} \right)^{1/2}, \quad \cos 2\zeta = \pm y \left(\frac{1 - x^2 \operatorname{tg}^2 \alpha}{y^2 - x^2} \right)^{1/2}, \\ x = (2\rho)^{-1} \{ 1 + p^2 - s^2 \pm [(1 + p^2 - s^2)^2 - 4p^2]^{1/2} \}, \quad y = s^{-1} (px - 1), \\ p = \eta/\gamma, \quad s = (\beta_5 - \beta_3)/\gamma. \end{aligned}$$

For such values of ρ , ζ expression (23) is equal to

$$\begin{aligned} \beta_1 (\cos^2 \omega - \sin^2 \omega \cos 2\alpha)^2 + \frac{\beta_4}{2} \sin^4 \omega \sin^2 2\alpha \\ + 2\gamma \cos^4 \omega + \sin^4 \omega \left(\frac{1 + \cos^2 2\alpha}{4} C \pm \frac{\cos 2\alpha}{2} D \right), \end{aligned} \quad (24)$$

where

$$C = 2\beta_4 + 4\beta_3 \beta_5 / \gamma, \quad D = 4\{ \beta_3 \beta_5 [\beta_4^2 - (\beta_3 - \beta_5)^2] \}^{1/2} / \gamma.$$

The extremum of expression (24) with respect to the angle α corresponds to

$$\cos 2\alpha = (4\beta_1 \operatorname{ctg}^2 \omega \pm D) / (2\beta_4 - 4\beta_1 - C). \quad (25)$$

Finally varying with respect to ω we have three solutions: 1) $\cos \omega = 0 \rightarrow \eta$ -phase (Ref. 8) and 2), 3)

$$\cos 2\omega = -2(2\beta_1 \gamma + \beta_3 \beta_5) \{ \beta_1 (C + 4\gamma \pm D) + 6\beta_3 \beta_5 \}^{-1}. \quad (26)$$

The quantity χ is then given by the expression

In the first case we find the polar, the planar, and the B -phase; in the second a new ι -phase

$$\varphi = \frac{\pi}{4}, \quad \operatorname{tg}^2 \theta = 2 \frac{\beta_1 + \gamma}{2\beta_1 + \gamma}, \quad \frac{\tau}{\chi} = \beta_2 + \gamma \frac{3\beta_1 + 2\gamma}{4\beta_1 + 3\gamma}. \quad (29)$$

Finally, in the last case we find the δ -phase of Ref. 6.

Let now $A = 0$. We get from Eq. (10.II)

$$(\chi_{xx} - \chi_{yy}) b_z = (\chi_{yy} - \chi_{zz}) b_x = (\chi_{xx} - \chi_{zz}) b_y = 0,$$

so that either $b_z \neq 0$, $b_x = b_y = 0$ and $\chi_{xx} = \chi_{yy}$; or else $\mathbf{b} = 0$. In the first case it follows from the z -component of Eqs. (10.VI, VII) that $B_{zz} = A_{zz} = 0$ so that (as $B = A = 0$) $B_{xx} = -B_{yy}$ and $A_{xx} = -A_{yy}$. Using the free rotation around the z -axis ($\chi_{xx} = \chi_{yy}$) we put $B_{xy} = 0$ and it then follows from the xy -component of Eq. (10.IV) that $A_{xx} = A_{yy}$, and since $A_{xx} = -A_{yy}$, we have $A_{xx} = A_{yy} = 0$. Adding and subtracting Eqs. III_{xy} and IV_{xx}, III_{xz} and IV_{yz}, III_{yz} and IV_{xz}, VI_x and VII_y, VI_y and VII_x of the set (10) we get

$$(\beta_2 \chi - \tau + 2\gamma \chi_{xx} \pm 2\mu b_z) (A_{xy} \pm B_{xx}) = 0, \quad (30)$$

$$(|A_{xz} \pm B_{yz}| + |A_{yz} \mp B_{xz}|) (|\beta_2 \chi - \tau + \gamma (\chi_{xx} + \chi_{zz}) \mp \mu b_z| + |\nu (\chi_{zz} - \chi_{xx}) \pm \eta b_z|) = 0.$$

Hence we have ($b_z \neq 0$) 4 cases:

- 1) $A_{xy} = B_{xx} = A_{xz} = A_{yz} = B_{xz} = B_{yz} = 0$,
- 2) $A_{xy} = B_{xx} = 0$, $A_{xz} = B_{yz} \neq 0$, $A_{yz} = -B_{xz} \neq 0$,
- 3) $A_{xy} = B_{xx} \neq 0$, $A_{yz} = B_{xz} = A_{xz} = B_{yz} = 0$,
- 4) $A_{xy} = B_{xx} \neq 0$, $A_{xz} = B_{yz} \neq 0$, $A_{yz} = -B_{xz} \neq 0$.

In the last case the set (30) reduces to three equations which are incompatible with the condition $b_z \neq 0$

$$\beta_2 \chi - \tau + 2\gamma \chi_{xx} + 2\mu b_z = 0, \\ \beta_2 \chi - \tau + \gamma (\chi_{xx} + \chi_{zz}) - \mu b_z = 0, \quad \nu (\chi_{zz} - \chi_{xx}) + \eta b_z = 0.$$

Subtracting the second equation from the first we get

$$\gamma (\chi_{xx} - \chi_{zz}) + 3\mu b_z = 0,$$

which together with the third equation gives $b_z = 0$.

In the case 1) $A_{ik} = B_{ik} = 0$ we find easily from Eqs. (10.I_{zz} and V_z) $(\beta_2 \chi - \tau + \beta_4 + \beta_5) \cdot \chi_{zz} = 0$, $\beta_2 \chi - \tau + \beta_4 (\chi - \chi_{zz}) = 0$ two solutions: the γ -phase (when $\chi_{zz} = 0$) and

$$\tau/\chi = \beta_2 + \beta_4 (\beta_4 + \beta_5) / (2\beta_4 + \beta_5). \quad (*)$$

In the case 2) $A_{xy} = B_{xx} = 0$, $A_{xz} = B_{yz} = 0$, $A_{yz} = -B_{xz}$. Using the freedom of rotation around the z -axis we put $A_{yz} = 0$. We write down Eqs. I_{xx}, IV_{yz}, V_z, VII_x of (10)

$$\begin{aligned} \text{I } (\beta_2 \chi - \tau) \chi_{xx} + \beta_3 B_{yz}^2 + (\beta_4 + \beta_5) \chi_{xx}^2 + (\beta_4 - \beta_5) b_z^2 &= 0, \\ \text{II } \beta_2 \chi - \tau + \gamma (\chi_{xx} + \chi_{zz}) - \mu b_z &= 0, \\ \text{III } (\beta_2 \chi - \tau + 2\beta_4 \chi_{xx}) b_z - \beta_3 B_{yz}^2 &= 0, \\ \text{IV } \nu (\chi_{zz} - \chi_{yy}) + \eta b_z &= 0. \end{aligned} \quad (31)$$

Adding Eqs. I and II of the set (31) we get

$$(\chi_{xx} + b_z) \{\beta_2 \chi - \tau + (\beta_4 + \beta_5) \chi_{xx} + (\beta_4 - \beta_5) b_z\} = 0, \quad (32)$$

after which we easily find two solutions of the set (31)

$$1) \frac{\tau}{\chi} = \beta_2 + (\beta_4^2 + \beta_4 \beta_5 - \beta_5^2) / (2\beta_4 + \beta_5 - 2\beta_3), \quad (33)$$

$$2) \tau/\chi = \beta_2 + (\eta\gamma^2 + 3\eta\gamma\nu + 3\mu\nu\gamma + \nu^2\mu) / (2(\eta\gamma + 3\mu\nu + 2\eta\nu)), \quad (*)$$

In the case 3) $A_{yz} = B_{xz} = A_{xz} = B_{yz} = 0$, $A_{xy} = B_{xx} \neq 0$ and

$$\beta_2 \chi - \tau + 2\gamma \chi_{xx} + 2\mu b_z = 0 \quad (34a)$$

[see (30)] and the unused equations of the set (10), (I_{xx}, I_{zz}, V_{zz}), reduce to the following:

$$\begin{aligned} (\beta_2 \chi - \tau) \chi_{xx} + 2\beta_3 B_{xx}^2 + (\beta_4 + \beta_5) \chi_{xx}^2 + (\beta_4 - \beta_5) b_z^2 &= 0, \\ \chi_{zz} \{\beta_2 \chi - \tau + (\beta_4 + \beta_5) \chi_{zz}\} &= 0, \\ \{\beta_2 \chi - \tau + \beta_4 (\chi - \chi_{zz})\} b_z + 2\beta_3 B_{xx}^2 &= 0. \end{aligned} \quad (34b)$$

Subtracting the last from the first equation we get

$$(\chi_{xx} - b_z) [\beta_2 \chi - \tau + (\beta_4 + \beta_5) \chi_{xx} + (\beta_4 - \beta_5) b_z] = 0.$$

In agreement with this equation and the second equation of the set (34b) we easily get four solutions of the set (34):

1) A -phase,

2) ε -phase of Ref. 7,

$$3) \tau/\chi = \beta_2 + (\beta_4^2 + \beta_4 \beta_5 - \beta_5^2) / (2\beta_4 + \beta_5 - 2\beta_3), \quad (35)$$

$$4) \frac{\tau}{\chi} = \beta_2 + \frac{(\beta_4 + \beta_5) (\beta_3 \beta_4 + \beta_4^2 - \beta_5^2)}{2\beta_3 \beta_4 - \beta_3 \beta_5 + 3\beta_4^2 - 3\beta_5^2}. \quad (*)$$

We note that Eq. (35) and the previously found Eq. (33) change into each other under the substitution $\beta_3 \rightleftharpoons \beta_5$. According to the selection rule formulated above these solutions can be solutions of the set (2). Using the restrictions on the contractions with respect to the spin indexes we can establish in these cases the form of the $\psi_{i\alpha}$ matrix. Thus, we have for the solution (33)

$$\chi^{1/2} \begin{pmatrix} \sin \theta & -i \sin \theta & 0 \\ i \sin \theta & \sin \theta & 0 \\ \cos \theta & i \cos \theta & 0 \end{pmatrix}. \quad (36a)$$

This matrix is, indeed, a solution of the set (2) when

$$\operatorname{tg}^2 \theta = (\beta_4 + \beta_5 - \beta_2) / 2(\beta_4 - \beta_5). \quad (36b)$$

We call it the κ -phase, while the solution obtained from it through the substitution $\beta_3 \rightleftharpoons \beta_5$ and the interchanging of the spin and orbital indexes is called the λ -phase.

We consider finally the last case $A = 0$, $\mathbf{b} = 0$. We can then write Eqs. (10.III, IV, VI, VII) in the form of the following relations:

$$\begin{aligned} (|\beta_2 \chi - \tau + \gamma (\chi_{xx} + \chi_{yy})| + |\chi_{xx} - \chi_{yy}|) (|A_{xy}| + |B_{xy}|) &= 0, \\ |\beta_2 \chi - \tau + 2\gamma \chi_{xx}| (|A_{xx}| + |B_{xx}|) &= 0, \end{aligned} \quad (37)$$

and the others are obtained from these through cyclic permutation, $x \rightarrow y \rightarrow z$. When $A = 0$ there are three cases

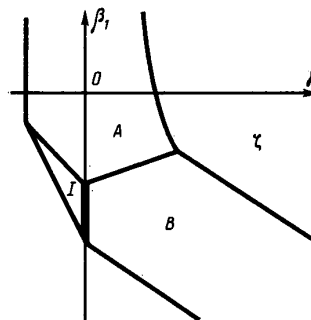


FIG. 1.

$$\begin{aligned}
& 1) A_{ik} = B_{ik} = 0, \\
& 2) \chi_{xx} = \chi_{yy}, A_{zi} = B_{zi} = 0, \beta_2 \chi - \tau + 2\gamma \chi_{xx} = 0, \\
& 3) \chi_{xx} = \chi_{yy} = \chi_{zz}, \tau \chi^{-1} = \beta_2 + 2\gamma/3 \\
& \quad - \text{this is the } \alpha\text{-phase of Ref. 7.}
\end{aligned} \tag{38}$$

In case 1) we find from Eqs. (10.I)

$$\begin{aligned}
& \chi_{xx} \{ \beta_2 \chi - \tau + (\beta_4 + \beta_5) \chi_{xx} \} \\
& = \chi_{yy} \{ \beta_2 \chi - \tau + (\beta_4 + \beta_5) \chi_{yy} \} = \chi_{zz} \{ \beta_2 \chi - \tau + (\beta_4 + \beta_5) \chi_{zz} \} = 0
\end{aligned}$$

the β -phase of Ref. 7 and two redundant solutions:

$$\tau/\chi = \beta_2 + (\beta_4 + \beta_5)/2, \quad \tau/\chi = \beta_2 + (\beta_4 + \beta_5)/3. \tag{*}$$

In case 2) from Eq. (38) and the zz -component of (10.I)

$$\chi_{zz} \{ \beta_2 \chi - \tau + (\beta_4 + \beta_5) \chi_{zz} \} = 0$$

we find the bipolar phase of Ref. 6 and

$$\tau/\chi = \beta_2 + 2\gamma(\beta_4 + \beta_5)/(2\gamma + \beta_4 + \beta_5). \tag{*}$$

One verifies easily that amongst the solutions indicated by (*) there are no partners changing into one another under the substitution $\beta_3 \leftrightarrow \beta_5$.

There are thus 18 extrema of the energy (1). We note that one of the five new solutions (Θ^+ , Θ^- , l , κ , λ) the κ -phase [see (36a,b) and (33)] has the lowest energy at the values $\beta_1 = 0.373$; $\beta_3 = 0.02$; $\beta_4 = 0.433$ and $\beta_5 = 0.677$ indicated by Barton and Moore at the end of Ref. 7. The quantity τ/χ in (33) is then equal to $\beta_2 + 0.3195$; for the ζ -phase which is closest in energy $\tau/\chi = \beta_2 + 0.3201$.

As we know now all the solutions of the equilibrium Eqs. (2) we can construct the phase diagram in the $\beta_1, \beta_2, \beta_3, \beta_4, \beta_5$ parameter space. It is convenient to show the phase diagram in the (β_1, γ) plane for different values of the parameters $\beta_2, \beta_4, \beta_3 - \beta_5$. As an example we give the diagram for the case of a possible coexistence of the A - and B -phases (see the figure). In the region below and to the left, the terms of fourth order in ψ in the energy are not positive-definite. The phase I is the polar phase; the fourth phase in the diagram is the ζ -phase of Ref. 7.

We note that in the analogous problem of the phases, when there is p -pairing in the two-dimensional case, and the orbital index takes on only two values (x, y) for the ψ -functions $\psi_{i\alpha}$ while the energy has the same form (1), the solutions are clearly the same as the three-dimensional ones in which there are no non-zero components in one "orbital" row. Altogether there are nine such solutions: the planar, polar, bipolar, $A, B, \gamma, \delta, \eta$, and λ -phases.

2. To study the stability of the solutions we need find the region where the energy increment F_2 , which is quadratic in arbitrary small deviations $\xi_{i\alpha}$ of the ψ -functions from the solutions, is positive definite

$$\begin{aligned}
F_2 = & -\tau \xi_{i\alpha} \xi_{i\alpha}^* + \frac{\beta_1}{2} (\psi_{i\alpha} \psi_{i\alpha} \xi_{j\beta} \xi_{j\beta}^* + 4\psi_{i\alpha} \xi_{i\alpha} \psi_{j\beta} \xi_{j\beta}^* \\
& + \xi_{i\alpha} \xi_{i\alpha} \psi_{j\beta} \psi_{j\beta}^*) \\
& + \frac{\beta_2}{2} (2\psi_{i\alpha} \psi_{i\alpha} \xi_{j\beta} \xi_{j\beta}^* + \psi_{i\alpha} \xi_{i\alpha} \psi_{j\beta} \xi_{j\beta}^* \\
& + \xi_{i\alpha} \psi_{i\alpha} \xi_{j\beta} \psi_{j\beta}^* + 2\psi_{i\alpha} \xi_{i\alpha} \xi_{j\beta} \psi_{j\beta}^*) \\
& + \frac{\beta_3}{2} (2\psi_{i\alpha} \psi_{i\beta} \xi_{j\alpha} \xi_{j\beta}^* + \xi_{i\alpha} \psi_{i\beta} \xi_{j\alpha} \psi_{j\beta}^*
\end{aligned}$$

$$\begin{aligned}
& + \psi_{i\alpha} \xi_{i\beta} \psi_{j\alpha} \xi_{j\beta}^* + 2\psi_{i\alpha} \xi_{i\beta} \xi_{j\alpha} \psi_{j\beta}^*) \\
& + \frac{\beta_4}{2} (2\psi_{i\alpha} \psi_{i\beta} \xi_{j\alpha} \xi_{j\beta}^* + 2\psi_{i\alpha} \xi_{i\beta} \psi_{j\alpha} \xi_{j\beta}^* \\
& + \psi_{i\alpha} \xi_{i\beta} \xi_{j\alpha} \psi_{j\beta}^* + \xi_{i\alpha} \psi_{i\beta} \psi_{j\alpha} \xi_{j\beta}^*) \\
& + \frac{\beta_5}{2} (\psi_{i\alpha} \psi_{i\beta} \xi_{j\alpha} \xi_{j\beta}^* + \xi_{i\alpha} \xi_{i\beta} \psi_{j\alpha} \psi_{j\beta}^* \\
& + 2\psi_{i\alpha} \xi_{i\beta} \xi_{j\alpha} \psi_{j\beta}^* + 2\psi_{i\alpha} \xi_{i\beta} \psi_{j\alpha} \xi_{j\beta}^*).
\end{aligned} \tag{39}$$

Here $\psi_{i\alpha}$ is a solution of Eqs. (2). For instance, for the B -phase

$$\psi_{i\alpha} = (\chi/3)^{1/2} \delta_{i\alpha}, \quad \chi = \tau(\beta_1 + \beta_2 + 2\gamma/3)^{-1/2}$$

we write the deviation $\xi_{i\alpha}$ in the form

$$\xi_{i\alpha} = \omega_{i\alpha} + i\varepsilon_{i\alpha} + e_{i\alpha j}(\mu_j + i\nu_j),$$

where $\omega_{i\alpha}$ and $\varepsilon_{i\alpha}$ are symmetric real tensors while μ_j and ν_j are real vectors. The quadratic form (39) then equals

$$\begin{aligned}
& \frac{4}{3} \chi \gamma \left(\omega_{i\alpha} - \frac{\omega}{3} \delta_{i\alpha} \right)^2 + \frac{2}{3} \frac{\tau}{\chi} \omega^2 - 2\chi \beta_1 \left(\varepsilon_{ik} - \frac{\varepsilon}{3} \delta_{ik} \right)^2 \\
& + \frac{2}{3} (2\beta_4 - 2\gamma - 3\beta_1) \nu_i^2,
\end{aligned} \tag{40}$$

where $\omega = \omega_{ii}$ and $\varepsilon = \varepsilon_{ii}$. The energy (14) is independent of the trace of the tensor ε_{ik} and of the vector μ_i since these quantities, clearly, call in the B -phase for a change in the ψ -function under a small gauge transformation ($\propto \varepsilon$) and small rotations ($\propto \mu_i$) of the spin or the orbital spaces. The stability conditions that follow from (40) for the B -phase are the same as the necessary stability conditions found by Jones.⁸ In the A -phase we find $\beta_3 < 0$, $\beta_3 + \beta_4 - \beta_5 < 0$, $\beta_1 + \beta_5 > 0$, and $\beta_2 + \beta_3 + \beta_4 > 0$.

There is an incorrect statement in Ref. 8, that the solution corresponding to the α -phase of Ref. 7 is unstable. The exact stability conditions reduce to the following inequalities:

$$\beta_1 > 0, \quad \gamma > 0, \quad \gamma + 3\beta_2 > 0, \quad \beta_4 > (\beta_3^2 + \beta_5^2 - \beta_3\beta_5)^{1/2}.$$

We note that the stability study is appreciably simplified if we eliminate from the arbitrary deviations $\xi_{i\alpha}$ the motions

$$\xi_{i\alpha} = i\psi_{i\alpha} \delta\varphi + \psi_{j\alpha} e_{ijk} \delta\theta_k + \psi_{i\beta} e_{\alpha\beta\gamma} \delta\omega_\gamma,$$

which reduce to small gauge transformations and rotations of the orbital and spin spaces.

We finally draw attention to one interesting fact. In the complete phase diagram there are two kinds of neighborhoods between phases. Firstly, there are lines (such as the boundary between the A - and B -phases) which are normal first-order phase transitions and correspond to a normal critical point in the (P, T) diagram. Secondly, there are unusual lines such as the boundary between the B - and the polar phase. It is clear from (14) that the B -phase loses its stability on that line ($\gamma = 0$). On the other hand, one verifies easily that the stability conditions for the polar phase are $\beta_1 + \beta_2 + \gamma > 0$, $\beta_1 + \beta_5 < 0$, $\beta_1 + \beta_3 < 0$, $2\beta_1 + \gamma < 0$, and $\gamma < 0$, i.e., it is also unstable when $\gamma = 0$. As the matrices that specify both solutions have the form

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

it is clear that the transition considered cannot be of second order. When $\gamma = 0$ the energies of these phases are equal to the energies of the planar phase and the ξ -phase of Ref. 7 and the solution found by Jones.⁸ All the solutions reduce for $\gamma = 0$ to real diagonal matrices. One checks easily that for $\gamma = 0$ there is a degenerate solution of the form

$$\begin{pmatrix} \sin \theta \sin \varphi & 0 & 0 \\ 0 & \sin \theta \cos \varphi & 0 \\ 0 & 0 & \cos \theta \end{pmatrix}$$

with arbitrary θ and φ . The situation is thus completely analogous to the orientation transitions in magnetics.

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¹Equation (5) has no antisymmetric real part.

²We note that in Eq. (57) of Ref. 7 we must replace $\cos^2 \varphi$ by $\cos 2\varphi$.

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