The structural distortion in antiferromagnetic LaFeAsO investigated by a group-theoretical approach

Ekkehard Krüger and Horst P. Strunk
Institut für Materialwissenschaft, Materialphysik, Universität Stuttgart, D-70569 Stuttgart, Germany
(Dated: January 18, 2013)

As experimentally well established, undoped LaFeAsO is antiferromagnetic below 137K with the magnetic moments lying on the Fe sites. We determine the orthorhombic body-centered group Imma (74) as the space group of the experimentally observed magnetic structure in the undistorted lattice, i.e., in a lattice possessing no structural distortions in addition to the magnetostriction. We show that LaFeAsO possesses a partly filled “magnetic band” with Bloch functions that can be unitarily transformed into optimally localized Wannier functions adapted to the space group Imma. This finding is interpreted in the framework of a nonadiabatic extension of the Heisenberg model of magnetism, the nonadiabatic Heisenberg model. Within this model, however, the magnetic structure with the space group Imma is not stable but can be stabilized by a (slight) distortion of the crystal turning the space group Imma into the space group Pmm2 (34). This group-theoretical result is in accordance with the experimentally observed displacements of the Fe and O atoms in LaFeAsO as reported by Clarina de la Cruz et al. [nature 453, 899 (2008)].

Keywords: magnetism, nonadiabatic Heisenberg model, group theory

I. INTRODUCTION

Undoped LaFeAsO undergoes an abrupt structural distortion from tetragonal to orthorhombic [1,3] or to monoclinic [4] symmetry at \( \sim 155 \)K as well as an antiferromagnetic spin ordering transition at \( \sim 137 \)K [1,4]. Clarina de la Cruz et al. [4] studied with high accuracy the structural distortion of LaFeAsO at 4K by neutron-scattering experiments and found the Fe and O atoms to be slightly shifted from their positions in the tetragonal phase. In agreement with the space group \( P4/nmm \), the \( z \) coordinates of iron and oxygen are exactly \( z = 1/2 \) and \( z = 0 \), respectively, in the tetragonal phase. The values \( \Delta z \) of the displacements at 4K in \( \pm z \) direction are reported to \( \Delta z = 0.0006 \) and \( \Delta z = 0.0057 \) for the iron and oxygen atoms, respectively [4]. These displacements cannot be simply explained by magnetostriction.

In the framework of a nonadiabatic extension of the Heisenberg model [5], called nonadiabatic Heisenberg model (NHM) [6–8], the magnetic order and the low-temperature structural distortion in LaFeAsO may be understood by group-theoretical methods. While the non-magnetic distortion of LaFeAsO between 155K and 137K shall be discussed in a following paper in the context of the superconducting state in the doped material, the present paper investigates the magnetic structure and the associated structural distortions below 137K.

In Sec. [III] we shall determine the space group \( S \) of the experimentally observed magnetic structure in LaFeAsO under the assumption that there are no distortions in addition to the magnetostriction. We shall show that \( S \) is compatible with the symmetry of the Bloch functions of the energy band of LaFeAsO denoted in Fig. [I] by the bold line. In the following Sec. [IV] we will ask whether \( S \) may be the space group of a stable magnetic structure, and in Sec. [V] we shall present the concept of “allowed space groups”. Finally, in Sec. [VI] we shall propose that the experimentally observed distortions of the crystal correspond to a change from the non-allowed space group \( S \) of the undistorted crystal to an allowed space group.

The NHM does not distinguish between orbital and spin moments. Therefore, we always speak of “magnetic moments” which may consist of both orbital and spin moments.

II. COORDINATE SYSTEMS

The coordinates systems used in this paper are depicted in Figs. [2] and [3] First, we use the \( x, y, z \) coordinate systems as depicted in Fig. [2] which coincides with the coordinates normally used in the literature on LaFeAsO, as, for instance, in the tables of Ref. [4]. This coordinate system defines the point group operations in the way described in Fig. [2]

In the following we shall consider three structures in pure LaFeAsO whose unit cells together with the basic translations \( T_1 \), \( T_2 \), and \( T_3 \) of the corresponding Bravais lattices are given in Fig. [3]. Fig. [3] (a) shows the tetragonal primitive Bravais lattice \( \Gamma_q \) of paramagnetic LaFeAsO above 155K which has the space group \( P4/nmm \) [1,11–15]. In Fig. [3] (b) the experimentally observed antiferromagnetic structure in a hypothetically undistorted crystal is depicted, which has the orthorhombic body-centered Bravais lattice \( \Gamma_0^s \) Finally, Fig. [3] (c) shows the antiferromagnetic structure in distorted LaFeAsO below 137K with the orthorhombic primitive Bravais lattice \( \Gamma_0 \).

For the description of these three structures we need to resort to three coordinate systems with unusual relationships. While the basic translations \( T_1 \), \( T_2 \), and \( T_3 \) are adapted to the respective structure, the origin of the \( x, y, z \) coordinate systems and the directions of its axes
relative to the atoms are fixed for all the three structures in Figs. III. Therefore, we may compare directly the space groups of the structures because the same point group operation in any structure is notated by the same symbol. As a consequence, the $A$ and $B$ axes (as given in Fig. II), but not the $x$ and $y$ axes, are perpendicular to each other in the orthorhombic structures. Furthermore, this choice of the $x$, $y$, $z$ axes requires a renaming of the point group operations given in the tables in the textbook of Bradley and Cracknell [16], as described in the notes to Tables I, II, and III.

III. THE UNDISTORTED MAGNETIC STRUCTURE

In this section we show that the experimentally observed magnetic structure in LaFeAsO is compatible with the symmetry of the Bloch functions of the magnetic band denoted in Fig. I by the bold line. First, in the following subsection we shall determine the magnetic group of the experimentally observed magnetic structure under the assumption that there are no structural distortions in the material in addition to the magnetostriction.

III.1. The experimentally determined magnetic structure and its magnetic group

We show that the group $Imma = \Gamma^v D_{2h}^{28}$ (74) with the orthorhombic body-centered Bravais lattice $\Gamma^v$ depicted in Fig. III (b) is the space group of the experimentally determined magnetic structure as it is given by Fig. 4 of Ref. I. In Fig. III (b) the unit cell of antiferromagnetic LaFeAsO is depicted where only the Fe atoms are indicated since the magnetic moments are localized on the Fe sites [1, 4]. This Fig. III (b) is identical with Fig. 4 of Ref. I because by application of the basic translations $T_1, T_2, T_3$ to the four Fe atoms in the unit cell the magnetic structure in Fig. 4 of Ref. I can be constructed.

In a first step we show that the positions of the atoms of LaFeAsO are invariant under the symmetry operations of $Imma$. They are clearly invariant under the translations of $Imma$ since its basic translations $T_1, T_2, T_3$ as given in Fig. III (b) are also translations of the paramagnetic structure depicted in Fig. III (a) [cf. the following relation (7)]. In order to show that the atoms of LaFeAsO are also invariant under the rotations and reflections of

FIG. 1. Band structure of tetragonal LaFeAsO as calculated by the FHI-aims program [9, 10], with symmetry labels determined by the authors. The symmetry labels can be identified from Table II see Appendix. The bold line shows the magnetic band (as defined in Sec. III.2) consisting of two branches.
axes, respectively. For instance, \(C_\text{origin}\) and being perpendicular to the \(A\) axis only in the tetragonal structure. The \(x, y, z\) axes and, in all the structures in Figs. 3 (a), (b), and (c), they have the direction of a lattice translation. Hence, in all the structures they are perpendicular to one another, while the \(z\) axis is perpendicular to the \(y\) axis only in the tetragonal structure. The \(z, A, B\) axes have the same positions in all the three structures in Figs. 3 (a), (b), and (c). The point group operations with the indices \(x, y, z\) are related to the depicted \(x, y, z, A, B\) and \(A\) axes, respectively. For instance, \(C_{4z}\) is a clockwise rotation of the lattice through \(\frac{\pi}{2}\) radians about the \(z\) axis, and \(C_{2a}\) is a rotation through \(\pi\) radians about the \(A\) axis. \(\sigma_{\text{d}} = IC_{2a}\) (\(I\) is the inversion) is a reflection in the plain containing the origin and being perpendicular to the \(A\) axis.

**Imma:** It is sufficient to consider the generating elements

\[
\{C_{2z}|0\frac{1}{2}\frac{1}{2}\},\{C_{2a}|\frac{1}{2}0\frac{1}{2}\},\{I|\frac{1}{2}\frac{1}{2}\}\tag{1}
\]

of **Imma** as they are given in Table 3.7 of Ref. [10]. However, in this paper they are written in the coordinate system defined by Figs. 2 and 3 (b), cf. the notes to Table II. We may easily compare the space group **Imma** with the paramagnetic space group \(P4/\text{nmnm}\) by writing the translations of the generating elements \(1\) in terms of the basic translations of the Bravais lattice \(\Gamma_q\) of \(P4/\text{nmnm}\) as depicted in Fig. 3 (a). Using the relation

\[
\begin{align*}
T_1 &\to T_1 + T_3 \\
T_2 &\to -T_1 + T_3 \\
T_3 &\to -T_2 - T_3.
\end{align*}
\]

(2)

[as derived from Figs. 3 (a) and (b)] we get the symmetry operations \(\{C_{2z}|\frac{1}{2}\frac{1}{2}\},\{C_{2a}|\frac{1}{2}0\frac{1}{2}\},\{I|001\}\), all of them being in the tetragonal space group \(P4/\text{nmnm}\), see the symmetry operations belonging to point \(\Gamma\) in Table II. Consequently, within the coordinate systems defined in Figs. 3 (a) and (b), the group **Imma** is a subgroup of \(P4/\text{nmnm}\). The important implication is that the positions of the atoms of LaFeAsO are invariant under the symmetry operations of **Imma**.

Now we can show that also the magnetic structure in Fig. 3 (b) is invariant under the generating elements \(1\) of **Imma:** One of the four Fe atoms in the unit cell lies at the position \(P_1 = \frac{1}{3}T_1 + \frac{1}{3}T_2 + \frac{1}{3}T_3\). Applying on this atom, e.g., the rotation \(C_{2z}\), we get an atom at the position \(P_2 = \frac{1}{3}T_1 - \frac{1}{3}T_2 + \frac{1}{3}T_3\) with the false direction of the magnetic moment. Then the associated translation \(t = \frac{1}{3}T_2 + \frac{1}{3}T_3\), however, moves this atom to the position \(P_3 = \frac{3}{2}T_1 + \frac{1}{2}T_2 + \frac{1}{2}T_3\) of an Fe atom with the correct direction of the magnetic moment. In the same way, it can be shown that the symmetry operation \(\{C_{2z}|0\frac{1}{2}\frac{1}{2}\}\) leaves invariant the directions of the magnetic moments of the three other Fe atoms in the unit cell. We get the same result for the other two generating elements \(\{C_{2a}|\frac{1}{2}0\frac{1}{2}\}\) and \(\{I|\frac{1}{2}\frac{1}{2}\}\). Consequently, the group **Imma** is the space group of the experimentally determined magnetic structure in LaFeAsO.

In addition, the magnetic structure depicted in Fig. 3 (b) is invariant under the anti-unitary operator \(\{K|\frac{1}{4}\frac{1}{4}0\}\), where \(K\) denotes the operator of time inversion. First, \(K\) reverses all the magnetic moments (and leaves invariant the positions of the atoms). Then the associated translation \(t = \frac{1}{3}T_1 + \frac{1}{3}T_2\) moves the Fe atoms to positions with the original directions of the magnetic moments. Also \(t\) leaves invariant the positions of the atoms because it is a lattice translation (namely \(T_3\)) in the paramagnetic lattice depicted in Fig. 3 (a). Hence, the magnetic group \(M\) of the experimentally determined magnetic structure in undistorted LaFeAsO as depicted in Fig. 3 (b) may be written as

\[
M = \text{Imma} + \{K|\frac{1}{4}\frac{1}{4}0\}\text{Imma}.
\]

(3)

**III.2. The symmetry of the Bloch functions of the magnetic band**

The energy band of LaFeAsO denoted in Fig. 1 by the bold line is characterized by the representations

\[
\begin{align*}
\Gamma^-_2, \Gamma^+_5: & X_1, X_1; M_3, M_4; A_3, A_2; Z^+_1, Z^-_5; R_1, R_1. \\
& \Gamma^-_2 \to \Gamma^-_3 \\
& M_3 \to X_3^+ + X_3^- \\
& A_3 \to \Gamma^+_3 + \Gamma^-_1 \\
& Z^+_1 \to X_1^+ \\
& R_1, X_1 \to T_1 + T_1.
\end{align*}
\]

(4)

(5)

Folding this energy band into the Brillouin zone of the space group **Imma** of the antiferromagnetic structure in the undistorted crystal depicted in Fig. 3 (b), the representations \(1\) of the Bloch functions transform as

\[
\begin{align*}
\Gamma^-_2 \to & \Gamma^-_3 \\
M_3 \to & X_3^+ + X_3^- \\
A_3 \to & \Gamma^+_3 + \Gamma^-_1 \\
Z^+_1 \to & X_1^+ \\
R_1, X_1 \to & T_1 + T_1.
\end{align*}
\]

(5)

see Table IV. The underlined representations form a band listed in Table V, namely band 2 in Table V (b). Hence, the Bloch functions of this band can be unitarily transformed into Wannier functions that are

- as well localized as possible,
FIG. 3. Coordinate systems and unit cells of three (magnetic) structures in LaFeAsO. For reasons of clarity, only the Fe atoms and in structure (c) also the O atoms are shown. $a$ and $c$ denote the lengths of the sides in the tetragonal unit cell. The coordinate systems define the symmetry operations \{R|pqr\} as used in this paper. They are written in the Seitz notation detailed in the textbook of Bradley and Cracknell [16]: $R$ stands for a point group operation and $pqr$ denotes the subsequent translation. The point group operation $R$ is related to the $x, y, z$ coordinate system as defined in Fig. 2 and $pqr$ stands for the translation $t = pT_1 + qT_2 + rT_3$ with the basic translations $T_i$ being different for the structures (a), (b), and (c). The origin of the coordinate systems is fixed for all the three structures (a), (b), and (c).

(a) The paramagnetic structure of LaFeAsO with the tetragonal space group $P4/nmm$ (129).
(b) The antiferromagnetic structure in the undistorted material with the orthorhombic space group $Imma$ (74).
(c) The antiferromagnetic structure in distorted LaFeAsO with the “allowed” orthorhombic space group $Pnn2$ (34). This paper proposes the indicated displacements of the Fe and O atoms in $z$ direction which are invariant under the magnetic group $M_{34} = Pnn2 + \{K|\pm \frac{1}{2}0\}Pnn2$. Since $Pnn2$ is a subgroup of $Imma$, the magnetic moments may have the same directions as in the undistorted structure (b). However, in the magnetic group $M_{34}$ the moments may also be canted within a plain perpendicular to the $z$ axis as depicted in Fig. 4.
— centered at the Fe atoms,
— and symmetry-adapted to the magnetic group \( M \) in Eq. \( \mathbf{3} \),

see the notes to Table \( \mathbf{V} \). For this reason, this band is called “magnetic band” related to the magnetic group \( M \). The NHM predicts that the electrons of this partly filled band may lower their Coulomb correlation energy by activating an exchange mechanism producing a magnetic structure with the magnetic group \( M \) and with the magnetic moments lying on the Fe sites, i.e., by producing the experimentally determined magnetic structure [6, 17, 18].

In this sense we say that the symmetry of the Bloch functions is “compatible” with the experimentally determined magnetic structure.

Table \( \mathbf{V} \) lists all the possible magnetic bands related to the magnetic group \( M \) in Eq. \( \mathbf{3} \). By this table one can make sure that the symmetry of the Bloch functions in relation (3) corresponds only to band 2 in Table \( \mathbf{V} \) (b). That is, the magnetic moments in LaFeAsO may only be situated at the Fe sites.

IV. STABILITY OF A MAGNETIC STRUCTURE

The magnetic band denoted in Fig. 1 by the bold line is related to the magnetic group \( M \) in Eq. \( \mathbf{3} \). However, this structure cannot exist in the undistorted material because the space group \( \text{Imma} \) does not possess suitable representations. This shall be substantiated in the following.

Let be

\[
M = S + \{K|t\}S
\] (6)

the magnetic group of a given antiferromagnetic structure, with \( S \) denoting the space group of this structure and \( \{K|t\} \) being an anti-unitary operator leaving invariant the magnetic structure. \( K \) still denotes the operator of time inversion.

The operator \( K \) reverses the magnetic moments in the antiferromagnetic ground state \( |G\rangle \), so

\[
|G\rangle = K|G\rangle
\] (7)

is the state with the opposite directions of the magnetic moments which clearly is different from \( |G\rangle \). Within the NHM, both states \( |\overline{G}\rangle \) and \( |G\rangle \) are eigenstates of a Hamiltonian denoted in Ref. [17] by \( \hat{H} \) which commutes with \( K \). Hence, \( |\overline{G}\rangle \) and \( |G\rangle \) belong to an irreducible two-dimensional corepresentation \( \tilde{D}^M \) of the group

\[
\tilde{M} = M + KM
\] (8)

of the Hamiltonian \( \hat{H} \), see Ref. [17], Sec. III.C.

However, when we restrict ourselves to the symmetry operations \( P \) of the subgroup \( M \) of \( \tilde{M} \), then \( \tilde{D}^M \) must subduce a one-dimensional corepresentation \( D^M \) of \( M \), that is,

\[
P|G\rangle = c \cdot |G\rangle \text{ for } P \in M,
\] (9)

where \( |c| = 1 \). In particular, this Eq. (9) is satisfied for the anti-unitary operator \( \{K|t\} \),

\[
\{K|t\}|G\rangle = c \cdot |G\rangle,
\] (10)

where still \( |c| = 1 \).

A stable magnetic state \( |G\rangle \) may exist if \( \tilde{M} \) possesses at least one suitable corepresentation \( \tilde{D}^M \). From this condition it follows the

Theorem IV.1 A stable magnetic state with the space group \( S \) can exist if \( S \) has at least one one-dimensional single-valued representation \( D \)

(i) following case (a) with respect to the magnetic group \( S + \{K|t\}S \) and

(ii) following case (c) with respect to the magnetic group \( S + KS \).

The cases (a) and (c) are defined in Eqs. (7.3.45) and (7.3.47), respectively, of Ref. [16]. They determine the dimension of the corepresentations of the magnetic groups \( S + \{K|t\}S \) and \( S + KS \), respectively, which are derived \(^{16} \) from the representation \( D \) of \( S \). The one-dimensional representation \( D \) may satisfy the second condition (ii) only if \( D \) has non-real characters.

This Theorem [IV.1] was proposed in Ref. [17] and written down in the present form in Ref. [19]. It can be understood following the theory of corepresentations as given in Sec. 7.3. of the textbook of Bradley and Cracknell [16]: Let \( D \) be a representation of \( S \) satisfying the first condition (i) of the theorem, then we may derive from \( D \) the one-dimensional corepresentation \( D^M \) of \( M \) given by Eq. (7.3.45) of Ref. [16] (with \( A = \{K|t\} \) and \( N = 1 \)).

Then we may derive from \( D^M \) the two-dimensional corepresentation \( \tilde{D}^M \) of \( \tilde{M} \) as it is given in Eq. (7.3.17) of Ref. [16], where now \( A = K \). [Bradley and Cracknell assume that the subgroup \( G \) in their Eq. (7.3.11) does not contain anti-unitary elements; for the derivation of their Eq. (7.3.17), however, these authors do not make use of this assumption.] If \( D \) satisfies additionally the second condition (ii) of the theorem, then the corepresentation \( \tilde{D}^M \) has just the required properties, cf. the Auxiliary Publication, citation 9, of Ref. [17].

In the present paper the cases (a) and (c) are determined (in Tables \( \mathbf{II} \) and \( \mathbf{III} \)) by the relatively straightforward equation (7.3.51) of Ref. [16],

\[
\sum_{B \in C} \chi(B^2) = \begin{cases} +|S| & \text{in case (a)} \\
-|S| & \text{in case (b)} \\
0 & \text{in case (c)} \end{cases}
\] (11)

The sum runs over the symmetry operations \( B \) in the left cosets \( C = \{K|t\}S \) and \( C = KS \), respectively, of
the magnetic groups. $\chi(B^2)$ is the character of $B^2$ in the representation $D$ and $|S|$ denotes, as usual, the order of $S$.

Table [II] shows that the space group $Imma$ does not possess one-dimensional representations with non-real characters. Consequently, all the one-dimensional representations of $Imma$ follow case (a) with respect to the magnetic group $Imma + KImma$ and hence, stable magnetic structures with the space group $Imma$ do not exist.

V. ALLOWED SPACE GROUPS IN ANTIFERROMAGNETIC LaFeAsO

As shown in the preceding Sec. [V], the magnetic structure depicted in Fig. 3(b) is not stable because its space group $Imma$ does not possess suitable representations. However, this structure may be stabilized by a (small) distortion of the crystal that turns the space group $Imma$ into a new space group possessing representations that allow the formation of a stable magnetic structure. This new space group shall be named an “allowed” space group in LaFeAsO. In this context we assume that the distortions of the crystal are so small that the magnetic structure in the distorted material differs hardly from the structure depicted in Fig. 3(b) because the symmetry of the Bloch functions of the magnetic band is compatible with the magnetic group $M$ in Eq. (3). For that reason we assume that the magnetic structure depicted in Fig. 3(b) is invariant under an allowed space group, i.e., we assume that an allowed space group is a subgroup of $Imma$.

In this section we look for all the allowed space groups in antiferromagnetic LaFeAsO by considering all the orthorhombic primitive and monoclinic primitive space groups in Table 3.7 of Ref. [16] with at least four point group elements. This is a laborious task because all the conceivable translations and rotations of the coordinate systems given in Table 3.7 of Ref. [16] should be regarded.

The coordinate system of the magnetic structure in LaFeAsO in an orthorhombic primitive or monoclinic primitive Bravais lattice is depicted in Fig. 3(c). The positions of the atoms and the magnetic structure are invariant under two anti-unitary operations of the form $\{K|a\}$, namely under $\{K|\frac{1}{2}\frac{1}{2}0\}$ and $\{K|00\frac{1}{2}\}$. Hence, we must look for space groups $S$ possessing one-dimensional representations following case (c) with respect to the magnetic group $S + KS$ and case (a) with respect either to $S + \{K|\frac{1}{2}\frac{1}{2}\frac{1}{2}\}S$ or to $S + \{K|00\frac{1}{2}\}S$, see Theorem [V,1].

We found the two allowed space groups $Pnn2 = \Gamma_o C14$ (34) and $P1 P1 P1 = \Gamma_o D3$ (19) and shall present them in the following two Secs. [V,1] and [V,2]. In Sec. [V,1] we will show that $Pnn2$ clearly is the space group of LaFeAsO.

V.1. The space group $Pnn2$

The space group $Pnn2$ has the orthorhombic-primitive Bravais lattice $\Gamma_o$ and can be defined by the two generating elements

$$\{\sigma_{da}|0\frac{1}{2}\frac{1}{2}\} \text{ and } \{\sigma_{db}|\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$$

(cf. Table 3.7 of Ref. [16] and the notes to Table III). The symmetry operations (12) are given in the coordinate systems of Fig. 3. As shown in the preceding Sec. IV, the magnetic structure in antiferromagnetic LaFeAsO by considering all the generating elements (12) in terms of the basic translations of the group $Imma$ as given in Fig. 3(b). Using the relation

$$\begin{align*}
T_1 & \rightarrow T_2 + T_3 \\
T_2 & \rightarrow T_1 + T_3 \\
T_3 & \rightarrow T_1 + T_2,
\end{align*}$$

$$\Gamma_o \rightarrow \Gamma_o$$

we get the operations $\{\sigma_{da}|\frac{1}{2}\frac{1}{2}\}$ and $\{\sigma_{db}|\frac{1}{2}\frac{1}{2}\}$, both belonging to the group $Imma$, see the symmetry operations belonging to point $\Gamma$ in Table III. Consequently, within the coordinate systems of Fig. 3 $Pnn2$ is a subgroup of $Imma$.

In contrast to the group $Imma$, the group $Pnn2$ possesses at point $S$ one-dimensional representations satisfying the conditions (i) and (ii) of Theorem [V,1] for the magnetic groups

$$M_{34} = Pnn2 + \{K|\frac{1}{2}\frac{1}{2}\frac{1}{2}\}Pnn2$$

and $Pnn2 + KPnn2$, respectively, see Table III. Further, the little group of $S$ comprises the whole space group. Hence, $Pnn2$ may be the space group of a stable magnetic structure. A stable antiferromagnetic ground state $|G\rangle$ is basis function of a one-dimensional corepresentation of $M_{34}$ and $|G\rangle$ and the time inverted state $\tilde{|G\rangle} = K|G\rangle$ form basis functions of an irreducible two-dimensional corepresentation of the group

$$\widetilde{M}_{34} = M_{34} + KM_{34}$$

which might be determined by Eq. (7.3.17) of Ref. [16]. [As an example, the analogous corepresentation for the spin-density-wave state in chromium is explicitly given in Ref. [17].]

V.2. The space group $P1P1P1$

A second allowed space group is the group $P1P1P1$ with the generating elements

$$\{C_{2a}|\frac{1}{2}\frac{1}{2}\frac{1}{2}\} \text{ and } \{C_{2b}|\frac{1}{2}\frac{1}{2}\frac{1}{2}\},$$

written again within the coordinate systems of Figs. 2 and 3(c). We do not describe this group but only report the result that a magnetic structure with the magnetic group

$$M_{19} = P1P1P1 + \{K|\frac{1}{2}\frac{1}{2}\frac{1}{2}\}P1P1P1$$

could be stable in LaFeAsO. However, antiferromagnetic LaFeAsO does not possess this space group, see the following Sec. [VI].
VI. DISTORTION OF THE CRYSTAL

The antiferromagnetic structure in undistorted LaFeAsO has the space group \textit{Imma}. Hence, in the undistorted antiferromagnetic material the nonadiabatic Hamiltonian \(H^n\) [as defined in Eq. (2.15) of Ref. [6]] would commute with all the symmetry operations of \textit{Imma}. However, as shown in the preceding sections, \textit{Imma} is not an allowed space group but has two allowed subgroups, namely \(Pnn2\) and \(P1P1P1\). Thus, either \(Pnn2\) or \(P1P1P1\), but not \textit{Imma} may be the space group of the antiferromagnetic structure in LaFeAsO. Consequently, the nonadiabatic Hamiltonian \(H^n\) commutes with the symmetry operations \(P\) of one of the allowed space groups \(S\), but does not commute with those symmetry operations that belong to \textit{Imma}, but do not belong to \(S\),

\[
\begin{align*}
[H^n, P] &= 0 \quad \text{for } P \in S, \\
[H^n, P] &\neq 0 \quad \text{for } P \in (\textit{Imma} - S). 
\end{align*}
\]

For that reason, the Fe and O atoms in LaFeAsO are slightly shifted from their positions in the space group \textit{Imma}.

In order to show this, we write the eight symmetry operations of \textit{Imma} as given in Table [III] for point \(\Gamma\) in terms of the basic translations \(T_1, T_2, \text{ and } T_3\) of the orthorhombic primitive lattice \(\Gamma_\alpha\) in Fig. [3](c),

\[
\begin{align*}
\{E|000\}, & \quad \{E|\frac{1}{2} \frac{1}{2} \frac{1}{2}\}, \\
\{C_{2z}|z00\}, & \quad \{C_{2z}|\frac{1}{2} \frac{1}{2} z\}, \\
\{C_{2y}|0y0\}, & \quad \{C_{2y}|\frac{1}{2} y 0\}, \\
\{C_{2x}|00z\}, & \quad \{C_{2x}|00\frac{1}{2}\}, \\
\{I|000\}, & \quad \{I|\frac{1}{2} \frac{1}{2} \frac{1}{2}\}, \\
\{\sigma_{x}z|0y0\}, & \quad \{\sigma_{x}z|y00\}, \\
\{\sigma_{y}a|00z\}, & \quad \{\sigma_{y}a|0z0\}, \text{ and } \\
\{\sigma_{y}a|z00\}, \text{ and } & \quad \{\sigma_{y}a|z00\}. 
\end{align*}
\]

(cf. relation [13]. For each symmetry operation from \(\Gamma_\alpha\) we get two operations in \(\Gamma_\beta\) because the operation \(\{E|\frac{1}{2} \frac{1}{2} \frac{1}{2}\}\) in \(\Gamma_\alpha\) is a lattice translation in \(\Gamma_\beta\) (\(E\) is the identity).

The antiferromagnetic structure with the space group \textit{Imma} is invariant under the sixteen symmetry operations [18] now written within the Bravais lattice \(\Gamma_\gamma\) of the structure in Fig. [3](c). By inspection of Fig. [3](c) we find under these sixteen operations four operations, namely

\[
\begin{align*}
\{E|000\}, & \quad \{C_{2z}|\frac{1}{2} 00\}, \\
\{\sigma_{x}a|00z\}, & \quad \{\sigma_{x}a|000\}, \text{ and } \\
\{\sigma_{y}a|\frac{1}{2} \frac{1}{2} \frac{1}{2}\}, & \quad \{\sigma_{y}a|\frac{1}{2} \frac{1}{2} \frac{1}{2}\}, 
\end{align*}
\]

leaving invariant the \textit{distorted} crystal as depicted in Fig. [3](c). These four operations form (together with the translations) a group, namely the allowed space group \(Pnn2\). Hence, the experimentally observed \(\beta\) displacements of the Fe and O atoms “realize” the space group \(Pnn2\) in the sense that they produce the correct commutation properties [given by Eq. (17)] of the nonadiabatic Hamiltonian \(H^n\) and stabilize in this way the magnetic structure in LaFeAsO. Together with the anti-unitary operator \(\{K|\frac{1}{2} \frac{1}{2} 0\}\) (which also leaves invariant the distorted structure), the symmetry operations [19] form the magnetic group \(M_{34}\) in Eq. (14).

In the magnetic group \(M_{34}\) the magnetic moments may be canted by two arbitrary angles \(\alpha\) and \(\beta\) as depicted in Fig. [3] (while such canted moments are not invariant under \textit{Imma}). Both angles are likely small because the symmetry of the Bloch functions of the magnetic band is compatible with the magnetic group \(M\) [in Eq. (3)] of the structure depicted in Fig. [3](b).

For the second allowed space group \(P1P1P1\), on the other hand, we have not found any simple distortion of the lattice realizing this group.

VII. CONCLUSIONS

Within the nonadiabatic Heisenberg model (NHM), the situation in the magnetic band of LaFeAsO (denoted in Fig. [1] by the bold line) is characterized by two different group-theoretical phenomena. On the one hand, the magnetic band (i.e., the symmetry of the Bloch func-
tions of this band) is related to the magnetic group $M$ of the experimentally observed magnetic structure in LaFeAsO and, on the other hand, any structure with the space group $M$ is unstable. These two phenomena are discussed in separated subsections VII.1 and VII.2.

VII.1. Nonadiabatic condensation energy

The nonadiabatic Heisenberg model (NHM) is defined by three postulates on the Coulomb correlation energy in narrow, partly filled bands $\Delta E$. A direct consequence of these postulates is the existence of the “nonadiabatic condensation energy” $\Delta E$ defined by Eq. (2.20) of Ref. [6]. The electrons at the Fermi level may lower their Coulomb correlation energy by $\Delta E$ by occupying an atomic-like state as defined by Mott [20] and Hubbard [21]: the electrons occupy localized states as long as possible and perform their band motion by hopping from one atom to another. In the present approach, the atomic-like state is consistently described in terms of symmetry-adapted and optimally localized Wannier functions and is precisely defined by an equation in the nonadiabatic system, namely by Eq. (2.19) of Ref. [6]. In case the considered partly filled band is a magnetic band related to a magnetic group $M$ (as considered in this paper), the electrons of this band may gain the energy $\Delta E$ by activating an exchange mechanism producing a magnetic structure with the magnetic group $M$ [6, 17, 18].

In former papers we could show that evidently the magnetic states in Cr [17], Fe [18], La$_2$CuO$_4$ [19], and YBa$_2$Cu$_3$O$_6$ [7] are connected with narrow, partly filled magnetic bands in the band structures of the respective materials. That is, there is evidence that the nonadiabatic condensation energy $\Delta E$ is responsible for the occurrence of the magnetic states in these materials. Also LaFeAsO possesses a magnetic band related to the magnetic group $M = Imma + \{K\{1110\}\}$ of the experimentally observed magnetic structure. This finding suggests that, first, the electrons of the magnetic band of LaFeAsO perform the atomic-like motion as defined within the NHM by Eq. (2.19) of Ref. [6] and that, secondly, the nonadiabatic condensation energy $\Delta E$ is responsible for the magnetic state.

VII.2. Stable magnetic structures

According to Theorem [V.3] not all the magnetic structures may be stable within the NHM. This theorem led already to an understanding of the really existing magnetic groups in Cr [17], La$_2$CuO$_4$ [19], and YBa$_2$Cu$_3$O$_6$ [7]. In the present paper, this theorem is the key for an understanding of the distortion (in addition to the magnetostriction) of antiferromagnetic LaFeAsO.

Theorem [V.3] defines “allowed” space groups belonging to stable magnetic structures. Though the magnetic band of LaFeAsO is related to the magnetic group $M = Imma + \{K\{1110\}\}$, the space group $Imma$ is not allowed. On the other hand, allowed space groups in LaFeAsO are the two groups $Pmn2$ and $P_{1}P_{1}P_{1}$. Consequently, the magnetic structure may be stabilized by a (slight) change of the atomic sites in such a way that the space group $Imma$ is turned into one of the allowed space groups. Briefly speaking, the structural distortion “realizes” the space group allowed in LaFeAsO.

The displacements of the Fe and O atoms as proposed in this paper are depicted in Fig. 3 (c). They have the space group $Pmn2$ and realize exactly this allowed space group. These displacements coincide in essence with the theoretically determined [22] and experimentally observed [4] structural distortions of LaFeAsO.

However, we could not confirm the space groups $Cmmn$ and $P112n$ as they have been reported for the space group of antiferromagnetic LaFeAsO in the undistorted [1] and the distorted [4] crystal, respectively. Nevertheless, using the space group $P112n$, Clarina de la Cruz et al. [4] discovered the important displacements of the Fe and O atoms in $z$ direction. The directions of the displacements depicted in Fig. 3 (c) do not essentially differ from those given in Table 2 of Ref. [4]: while they coincide absolutely within the Fe or O layers, Table 2 of Ref. [4] suggests that the displacements are periodic with $T_{3}/2$. As depicted in Fig. 3 (c), the displacements proposed in this paper alternate their directions at an interval of $T_{3}/2$. However, in the space group $Pmn2$ the amounts of the displacements in up and down direction may be principally different because they are not connected by symmetry operations.

ACKNOWLEDGMENTS

We wish to thank Volker Blum from the aims team of the Fritz-Haber-Institut der Max-Planck-Gesellschaft in Berlin for extending the aims program by an output of the eigenvectors which enabled us to determine the symmetry of the Bloch functions in the band structure of LaFeAsO. We are indebted to Franz-Werner Gergen from the EDV group of the Max-Planck-Institut für Metallforschung in Stuttgart for his assistance in getting to run the computer programs needed for this work, and we thank Ernst Helmut Brandt for valuable discussion and Ove Jepsen for initiating this paper.

1. T. Nomura, S. W. Kim, Y. Kamihara, M. Hirano, P. V. Sushko, K. Kato, M. Takata, A. L. Shluger, and H. Hosono, Supercond. Sci. Technol. 21, 125028 (2008).
2. S. Kitao, Y. Kobayashi, S. Higashitaniguchi, M. Saito, Y. Kamihara, M. Hirano, T. Mitsui, H. Hosono, and M. Seto, J. Phys. Soc. Japan 77, 103706 (2008).

3. Y. Nakai, K. Ishida, Y. Kamihara, M. Hirano, and H. Hosono, J. Phys. Soc. Japan 77, 073701 (2008).

4. C. de la Cruz, Q. Huang, J. W. Lynn, J. Li, W. R. II, J. L. Zarestky, H. A. Mook, G. F. Chen, J. L. Luo, N. L. Wang, and P. Dai, nature 453, 899 (2008).

5. W. Heisenberg, Z. Phys. 49, 619 (1928).

6. E. Krüger, Phys. Rev. B 63, 144403 (2001).

7. E. Krüger, Phys. Rev. B 75, 024408 (2007).

8. E. Krüger, J. Supercond. 23, 213 (2010).

9. V. Blum, R. Gehrke, F. Hanke, P. Havu, V. Havu, X. Ren, K. Reuter, and M. Scheffler, Computer Physics Communications 180, 2175 (2009).

10. V. Havu, V. Blum, P. Havu, and M. Scheffler, Computer Physics Communications 228, 8367 (2009).

11. Y. Kamihara, T. Watanabe, M. Hirano, and H. Hosono, J. Am. Chem. Soc. 130, 3296 (2008).

12. G. F. Chen, Z. Li, G. Li, J. Zhou, D. Wu, J. Dong, W. Z. Hu, P. Zheng, Z. J. Chen, H. Q. Yuan, J. Singleton, J. L. Luo, and N. L. Wang, Phys. Rev. Lett. 101, 057007 (2008).

13. X. H. Chen, T. Wu, G. Wu, R. H. Liu, H. Chen, and D. F. Fang, Nature 453, 761 (2008).

14. H.-H. Wen, G. Mu, L. Fang, H. Yank, and X. Zhu, Europhys. Lett. 82, 17009 (2008).

15. J. Dong, H. J. Zhang, G. Xu, Z. Li, G. Li, W. Z. Hu, D. Wu, G. F. Chen, X. Dai, J. L. Luo, Z. Fang, and N. L. Wang, Europhys. Lett. 83, 27006 (2008).

16. C. Bradley and A.P. Cracknell, The Mathematical Theory of Symmetry in Solids (Claredon, Oxford, 1972).

17. E. Krüger, Phys. Rev. B 40, 11090 (1989).

18. E. Krüger, Phys. Rev. B 59, 13795 (1999).

19. E. Krüger, J. Supercond. 18(4), 433 (2005).

20. N. F. Mott, Can. J. Phys. 34, 1356 (1956).

21. J. Hubbard, Proc. R. Soc. London, Ser. A 276, 238 (1963).

22. T. Yildirim, Phys. Rev. Lett. 101, 057010 (2008).

23. E. Krüger, Phys. Rev. B 32, 7493 (1985).

Appendix: Tables
TABLE I. Character tables of the single-valued irreducible representations of the space group $P4/nmm = \Gamma_q D_{4h}^7$ (129) of tetragonal paramagnetic LaFeAsO.

| $\Gamma(000)$, $Z(00\frac{1}{2})$ | \{E\{000\} | $C_{2x}\{0\|\frac{1}{2}\}$ | $C_{2y}\{0\|\frac{1}{2}\}$ | $C_{2z}\{000\}$ | $I\{000\}$ | $\sigma_z\{0\|\frac{1}{2}\}$ | $\sigma_y\{0\|\frac{1}{2}\}$ | $\sigma_d\{000\}$ |
|-----------------------------|-----------------------------|-----------------------------|-----------------------------|-----------------------------|-----------------------------|-----------------------------|-----------------------------|-----------------------------|
| $\Gamma^+_1$, $Z^+_1$      | 1                           | 1                           | 1                           | 1                           | 1                           | 1                           | 1                           | 1                           |
| $\Gamma^+_2$, $Z^+_2$      | 1                           | 1                           | 1                           | -1                          | -1                          | 1                           | 1                           | -1                          |
| $\Gamma^+_3$, $Z^+_3$      | 1                           | 1                           | -1                          | 1                           | 1                           | -1                          | 1                           | -1                          |
| $\Gamma^+_4$, $Z^+_4$      | 1                           | 1                           | -1                          | -1                          | 1                           | 1                           | -1                          | 1                           |
| $\Gamma^+_5$, $Z^+_5$      | 2                           | -2                          | 0                           | 0                           | 2                           | -2                          | 0                           | 0                           |
| $\Gamma^-_1$, $Z^-_1$      | 1                           | 1                           | 1                           | 1                           | -1                          | -1                          | -1                          | -1                          |
| $\Gamma^-_2$, $Z^-_2$      | 1                           | 1                           | 1                           | -1                          | -1                          | 1                           | 1                           | -1                          |
| $\Gamma^-_3$, $Z^-_3$      | 1                           | 1                           | -1                          | 1                           | -1                          | 1                           | 1                           | -1                          |
| $\Gamma^-_4$, $Z^-_4$      | 1                           | 1                           | -1                          | -1                          | 1                           | 1                           | -1                          | 1                           |
| $\Gamma^-_5$, $Z^-_5$      | 2                           | -2                          | 0                           | 0                           | 2                           | 0                           | 0                           | 0                           |

$M(\frac{1}{2}\frac{1}{2}0)$

| $\{E\{000\} | E\{010\} | \sigma_{da}\{\frac{1}{2}\|\frac{1}{2}\}$ | $\sigma_{da}\{\frac{1}{2}\|\frac{1}{2}\}$ | $I\{010\}$ | $\{E\{000\} | E\{010\} | \sigma_{da}\{\frac{1}{2}\|\frac{1}{2}\}$ | $\sigma_{da}\{\frac{1}{2}\|\frac{1}{2}\}$ | $I\{010\}$ |
|-----------------------------|-----------------------------|-----------------------------|-----------------------------|-----------------------------|-----------------------------|-----------------------------|-----------------------------|-----------------------------|
| $M_1$                       | 2                           | -2                          | 2                           | 2                           | 2                           | -2                          | 2                           | 0                           |
| $M_2$                       | 2                           | -2                          | -2                          | 2                           | 0                           | 0                           | 0                           | 0                           |
| $M_3$                       | 2                           | -2                          | -2                          | 2                           | 0                           | 0                           | 0                           | 0                           |
| $M_4$                       | 2                           | -2                          | -2                          | 2                           | 0                           | 0                           | 0                           | 0                           |

$M(\frac{1}{2}\frac{1}{2}0)$ (continued)

| $\{E\{000\} | E\{010\} | \sigma_{da}\{\frac{1}{2}\|\frac{1}{2}\}$ | $\sigma_{da}\{\frac{1}{2}\|\frac{1}{2}\}$ | $I\{010\}$ | $\{E\{000\} | E\{010\} | \sigma_{da}\{\frac{1}{2}\|\frac{1}{2}\}$ | $\sigma_{da}\{\frac{1}{2}\|\frac{1}{2}\}$ | $I\{010\}$ |
|-----------------------------|-----------------------------|-----------------------------|-----------------------------|-----------------------------|-----------------------------|-----------------------------|-----------------------------|-----------------------------|
| $\{\sigma_y\{0\|\frac{1}{2}\}$ | $\{C_{2x}\{\frac{1}{2}\|10\}$ | $\{C_{2y}\{0\|\frac{1}{2}\}$ | $\{S_{4x}\{\frac{1}{2}\}$ | $\{\sigma_y\{0\|\frac{1}{2}\} | \{C_{2x}\{\frac{1}{2}\|10\}$ | $\{C_{2y}\{0\|\frac{1}{2}\}$ | $\{S_{4x}\{\frac{1}{2}\}$ | $\{\sigma_y\{0\|\frac{1}{2}\}$ | $\{C_{2x}\{\frac{1}{2}\|10\}$ |
| $\{\sigma_x\{\frac{1}{2}\}$ | $\{C_{2y}\{0\|\frac{1}{2}\}$ | $\{\sigma_y\{\frac{1}{2}\}$ | $\{C_{2x}\{\frac{1}{2}\|10\}$ | $\{C_{2y}\{0\|\frac{1}{2}\}$ | $\{S_{4x}\{\frac{1}{2}\}$ | $\{\sigma_y\{0\|\frac{1}{2}\}$ | $\{C_{2x}\{\frac{1}{2}\|10\}$ |
| $\{\sigma_x\{\frac{1}{2}\}$ | $\{C_{2y}\{0\|\frac{1}{2}\}$ | $\{\sigma_y\{\frac{1}{2}\}$ | $\{C_{2x}\{\frac{1}{2}\|10\}$ | $\{C_{2y}\{0\|\frac{1}{2}\}$ | $\{S_{4x}\{\frac{1}{2}\}$ | $\{\sigma_y\{0\|\frac{1}{2}\}$ | $\{C_{2x}\{\frac{1}{2}\|10\}$ |

| $M_1$                       | 0                           | 0                           | 0                           | 0                           | 0                           | 0                           | 0                           | 0                           |
| $M_2$                       | 0                           | 2                           | -2                          | 0                           | 0                           | 0                           | 0                           | 0                           |
| $M_3$                       | 0                           | 0                           | 0                           | 0                           | 0                           | 0                           | 0                           | 0                           |
| $M_4$                       | 0                           | -2                          | 2                           | 0                           | 0                           | 0                           | 0                           | 0                           |
\[ A(\frac{1}{2} \frac{1}{2} \frac{1}{2}) \]

| \{E[000]\} | \{E[001]\} | \{C_{2\parallel} \frac{1}{2} \frac{1}{2} 0\} | \{C_{2\parallel} \frac{1}{2} \frac{1}{2} 1\} | \{\sigma_{d\alpha} \frac{1}{2} \frac{1}{2} 0\} | \{\sigma_{d\alpha} \frac{1}{2} \frac{1}{2} 1\} | \{I[001]\} |
|---|---|---|---|---|---|---|
| \(A_1\) | 2 | -2 | 2 | -2 | 2 | -2 | 0 |
| \(A_2\) | 2 | -2 | -2 | 2 | 0 | 0 | 0 |
| \(A_3\) | 2 | -2 | 2 | -2 | 2 | 0 | 0 |
| \(A_4\) | 2 | -2 | -2 | 2 | 0 | 0 | 0 |

\[ A(\frac{1}{2} \frac{1}{2} \frac{1}{2}) \text{ (continued)} \]

\[ \{\sigma_y \frac{1}{2} \frac{1}{2} 0\} | \{C_{2\parallel} \frac{1}{2} \frac{1}{2} 01\} | \{C_{2\parallel} \frac{1}{2} \frac{1}{2} 11\} | \{S_{4\parallel} \frac{1}{2} \frac{1}{2} 01\} | \{\sigma_y \frac{1}{2} \frac{1}{2} 0\} | \{C_{2\parallel} \frac{1}{2} \frac{1}{2} 01\} | \{C_{2\parallel} \frac{1}{2} \frac{1}{2} 11\} | \{S_{4\parallel} \frac{1}{2} \frac{1}{2} 00\} \]

| \{C_{2\parallel} \frac{1}{2} \frac{1}{2} 00\} | \{C_{2\parallel} \frac{1}{2} \frac{1}{2} 01\} | \{C_{2\parallel} \frac{1}{2} \frac{1}{2} 10\} | \{C_{2\parallel} \frac{1}{2} \frac{1}{2} 11\} | \{\sigma_x \frac{1}{2} \frac{1}{2} 00\} | \{\sigma_x \frac{1}{2} \frac{1}{2} 01\} | \{\sigma_x \frac{1}{2} \frac{1}{2} 10\} | \{\sigma_x \frac{1}{2} \frac{1}{2} 11\} | \{I[001]\} | \{\sigma_y \frac{1}{2} \frac{1}{2} 0\} |
|---|---|---|---|---|---|---|---|---|
| \(A_1\) | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| \(A_2\) | 0 | 2 | -2 | 0 | 0 | 0 | 0 | 0 |
| \(A_3\) | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| \(A_4\) | 0 | -2 | 2 | 0 | 0 | 0 | 0 | 0 |

\[ R(0 \frac{1}{2} \frac{1}{2}) \]

| \{E[000]\} | \{E[001]\} | \{C_{2\parallel} \frac{1}{2} \frac{1}{2} 0\} | \{C_{2\parallel} \frac{1}{2} \frac{1}{2} 1\} | \{\sigma_x \frac{1}{2} \frac{1}{2} 00\} | \{\sigma_x \frac{1}{2} \frac{1}{2} 01\} | \{\sigma_x \frac{1}{2} \frac{1}{2} 10\} | \{\sigma_x \frac{1}{2} \frac{1}{2} 11\} | \{I[001]\} | \{\sigma_y \frac{1}{2} \frac{1}{2} 0\} |
|---|---|---|---|---|---|---|---|---|
| \(R_1\) | 2 | -2 | 0 | 0 | 2 | -2 | 0 | 0 |
| \(R_2\) | 2 | -2 | 0 | 0 | 0 | -2 | 2 | 0 |

\[ X(0 \frac{1}{2} \frac{1}{2}) \]

| \{E[000]\} | \{E[010]\} | \{C_{2\parallel} \frac{1}{2} \frac{1}{2} 0\} | \{C_{2\parallel} \frac{1}{2} \frac{1}{2} 1\} | \{\sigma_x \frac{1}{2} \frac{1}{2} 00\} | \{\sigma_x \frac{1}{2} \frac{1}{2} 01\} | \{\sigma_x \frac{1}{2} \frac{1}{2} 10\} | \{\sigma_x \frac{1}{2} \frac{1}{2} 11\} | \{I[010]\} | \{\sigma_y \frac{1}{2} \frac{1}{2} 0\} |
|---|---|---|---|---|---|---|---|---|
| \(X_1\) | 2 | -2 | 0 | 0 | 2 | -2 | 0 | 0 |
| \(X_2\) | 2 | -2 | 0 | 0 | 0 | -2 | 2 | 0 |

Notes to Table I

(i) The space group operations are related to the coordinate systems in Figs. 2 and 3 (a).

(ii) The character table is determined from Table 5.7 of Ref. 16. The origin of the coordinate system used in Ref. 16 is translated into the origin used in this paper by \(t_0 = -\frac{1}{2} T_1 - \frac{1}{2} T_2\). That is, the symmetry operations \(P_{bc}\) given in Table 5.7 of Ref. 16 are changed into the operations \(P_0\) used in this paper by the equation

\[ P_0 = \{E[t_0]\} P_{bc} \{E[-t_0]\} \]

where \(E\) is the identity operation, cf. Eq. (3.5.11) of Ref. 16 (which is related to the opposite translation \(-t_0\)).
TABLE II. Character tables of the single-valued irreducible representations of the orthorhombic space group $Imma = \Gamma_0^a D_{2h}^{28}$ (74) of the antiferromagnetic structure depicted in Fig. 3(b).

$$\Gamma(000)$$

| $K$ | $\{E|000\}$ | $\{C_{2h}|00\frac{1}{2}\}$ | $\{C_{2h}|0\frac{1}{2}0\}$ | $\{I|\frac{1}{2}0\}$ | $\{\sigma_z|\frac{1}{2}0\}$ | $\{\sigma_{da}|0\frac{1}{2}\}$ | $\{\sigma_{da}|000\}$ |
|-----|-------------|----------------------------|-----------------------------|-----------------|------------------|-----------------|--------------------|
| $\Gamma_1^+$ (a) | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| $\Gamma_2^+$ (a) | 1 | -1 | 1 | -1 | 1 | -1 | 1 |
| $\Gamma_3^+$ (a) | 1 | 1 | -1 | 1 | 1 | -1 | -1 |
| $\Gamma_4^+$ (a) | 1 | -1 | 1 | -1 | -1 | 1 | 1 |
| $\Gamma_5^+$ (a) | 1 | 1 | -1 | -1 | 1 | -1 | -1 |
| $\Gamma_6^+$ (a) | 1 | 1 | 1 | -1 | -1 | 1 | 1 |

$$\Gamma(\pm \frac{1}{2} \pm \frac{1}{2} \pm \frac{1}{2})$$

| $K$ | $\{E|000\}$ | $\{C_{2h}|00\frac{1}{2}\}$ | $\{C_{2h}|0\frac{1}{2}0\}$ | $\{I|\pm \frac{1}{2}\pm \frac{1}{2}\}$ | $\{\sigma_z|\pm \frac{1}{2}\pm \frac{1}{2}\}$ | $\{\sigma_{da}|0\frac{1}{2}\}$ | $\{\sigma_{da}|000\}$ |
|-----|-------------|----------------------------|-----------------------------|-----------------|------------------|-----------------|--------------------|
| $\Gamma_1^+$ (a) | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| $\Gamma_2^+$ (a) | 1 | -1 | 1 | -1 | 1 | -1 | 1 |
| $\Gamma_3^+$ (a) | 1 | 1 | -1 | 1 | 1 | -1 | -1 |
| $\Gamma_4^+$ (a) | 1 | -1 | 1 | -1 | -1 | 1 | 1 |
| $\Gamma_5^+$ (a) | 1 | 1 | -1 | -1 | 1 | -1 | -1 |
| $\Gamma_6^+$ (a) | 1 | 1 | 1 | -1 | -1 | 1 | 1 |

$R(\pm \frac{1}{2}, 0, 0)$

| $K$ | $\{E|000\}$ | $\{C_{2h}|\frac{1}{2}00\}$ | $\{I|\frac{1}{2}\pm \frac{1}{2}\}$ | $\{\sigma_{da}|0\pm \frac{1}{2}\pm \frac{1}{2}\}$ |
|-----|-------------|----------------------------|-----------------|------------------|
| $R_1^+$ (a) | 1 | 1 | 1 | 1 |
| $R_2^+$ (a) | 1 | -1 | -1 | -1 |
| $R_3^+$ (a) | 1 | 1 | -1 | -1 |

$S(\pm \frac{1}{2}, 0, 0)$

| $K$ | $\{E|000\}$ | $\{C_{2h}|\pm \frac{1}{2}00\}$ | $\{I|\pm \frac{1}{2}\pm \frac{1}{2}\}$ | $\{\sigma_{da}|0\pm \frac{1}{2}\pm \frac{1}{2}\}$ |
|-----|-------------|----------------------------|-----------------|------------------|
| $S_1^+$ (a) | 1 | 1 | 1 | 1 |
| $S_2^+$ (a) | 1 | -1 | -1 | -1 |
| $S_3^+$ (a) | 1 | 1 | -1 | -1 |

Notes to Table II

(i) The points $T$ and $W$ are not listed because they possess only one two-dimensional representation $T_1$ and $W_1$, respectively.

(ii) The character tables are determined from Table 5.7 in Ref. [16]. The origin of the coordinate system used in Ref. [16] is translated into the origin used in this paper by $t_0 = \frac{1}{2} T_{10}$. That is, the symmetry operations $P_{bc}$ given in Table 5.7 of Ref. [16] are changed into the operations $P_b$ used in this paper by the equation

$$P_b = \{E|t_0\} P_{bc} \{E|-t_0\},$$

where $E$ is the identity operation, cf. Eq. (3.5.11) of Ref. [16] (which is related to the opposite translation $-t_0$).

(iii) The space group operations are related to the coordinate systems in Figs. 2(b) and 3(b). The $x$, $y$, and $z$ axes have the same orientations as in the tetragonal structure in Fig. 3(b). In this way, $Imma$ becomes a subgroup of the tetragonal group $P4/nmm$. As a consequence, the $xyz$ coordinate system used in Ref. [16] is rotated anti-clockwise with respect to the basic translations through $\frac{\pi}{4}$ radians about the $z$ axis. Thus, the $x$ and $y$ axes in Ref. [16] become the $B$ and $A$ axes, respectively, in this paper, see Fig. 2. Consequently, the point group operations belonging to the space group operations $P_b$ calculated by the above equation are renamed in a second step. For instance, the operation $C_{2h}$ in Table 5 of Ref. [16] turns into the operation $C_{2h}\prime$.

(iv) $K$ stands for the operator of time-inversion. The entries below $K$ specify whether the related representation follows, with respect to the magnetic group $Imma + KImma$, case (a), case (b), or case (c) when they are given by Eqs. (7.3.45-47) of Ref. [16].

(v) The cases (a), (b), and (c) are determined by Eq. [IV.1].

(vi) All the one-dimensional representations of the space group $Imma$ are real and, hence, follow case (a) with respect to $Imma + KImma$. Therefore, stable magnetic structures with this space group do not exist, see Theorem [IV.1].
Notes to Table III

(i) In addition to $\Gamma$ only the points $Z$ and $S$ are listed because only $Z$ and $S$ possess one-dimensional non-real representations.

(ii) The character tables are determined from Table 5.7 in Ref. [16]. The origin of the coordinate system used in Ref. [16] is translated into the origin used in this paper by $t_0 = \frac{1}{2}T_3$. That is, the symmetry operations $P_{bc}$ given in Table 5.7 of Ref. [16] are changed into the operations $P_b$ used in this paper by the equation

$$P_b = \{E|t_0\}P_{bc}\{E| - t_0\},$$

where $E$ is the identity operation, cf. Eq. (3.5.11) of Ref. [16] (which is related to the opposite translation $-t_0$).

(iii) The space group operations are related to the coordinate systems in Figs. 2 and 3 (c). The $x$, $y$, and $z$ axes have the same orientations as in the tetragonal structure in Fig. 2 (a). In this way, Pnn2 becomes a subgroup of the tetragonal group P4/nmm. As a consequence, the $xyz$ coordinate system used in Ref. [16] is rotated anti-clockwise with respect to the basic translations through $\frac{1}{4}$ radians about the $z$ axis. Thus, the $x$ and $y$ axes in Ref. [16] become the $B$ and $A$ axes, respectively, in this paper, see Fig. 2. Consequently, the point group operations belonging to the space group operations $P_b$ calculated by the above equation are renamed in a second step. For instance, the operation $\sigma_x$ in Table 5.7 of Ref. [16] turns into the operation $\sigma_{db}$.

(iv) $K$ stands for the operator of time inversion. The entries below $K$ and the operators $\{K|t\}$ specify whether the related representation follows, with respect to the magnetic groups Pnn2 + KPnn2 and Pnn2 + \{K|t\}Pnn2, respectively, case (a), case (b), or case (c) when they are given by Eqs. (7.3.45-47) of Ref. [16].

(v) The cases (a), (b), and (c) are determined by Eq. [11].

(vi) The little group of point $S$ comprises the whole space group Pnn2 and $S$ possesses one-dimensional representations following case (c) and case (a) with respect to Pnn2 + KPnn2 and Pnn2 + \{K|t\}Pnn2, respectively. Consequently, a magnetic structure with the space group Pnn2 can be stable, see Theorem [11].
TABLE IV. Compatibility relations between the Brillouin zone for tetragonal paramagnetic LaFeAsO and the Brillouin zone for the orthorhombic antiferromagnetic structure depicted in Fig. 3(b).

| Γ        | M1          | M2          | M3          | M4          |
|---------|-------------|-------------|-------------|-------------|
| Γ̂ ̄1  | X^+ + X^-3 | X^+ + X^-2 | X^+ + X^-1 | X^+ + X^-1 |
| Γ̂ ̄2  |             |             |             |             |
| Γ̂ ̄3  |             |             |             |             |
| Γ̂ ̄4  |             |             |             |             |
| Γ̂ ̄5  |             |             |             |             |

Notes to Table IV

(i) The antiferromagnetic structure in Fig. 3(b) has the space group Imma.

(ii) The Brillouin zone for the orthorhombic space group Imma lies within the Brillouin zone for the tetragonal space group P4/nmm. The points Γ and A in the tetragonal Brillouin zone are equivalent to the point Γ in the orthorhombic Brillouin zone; M and X are equivalent to X, and R and X are equivalent to T.

(iii) The upper rows list the representations of the little groups of the points of symmetry in the Brillouin zone for the tetragonal paramagnetic phase. The lower rows list representations of the little groups of the related points of symmetry in the Brillouin zone for the antiferromagnetic structure.

The representations in the same column are compatible in the following sense: Bloch functions that are basis functions of a representation D_i in the upper row can be unitarily transformed into the basis functions of the representation given below D_i.

(iv) The compatibility relations are determined in the way described in great detail in Ref. [23].

(v) The representations are labeled as given in Tables I and II respectively.
TABLE V. Single-valued representations of all the magnetic bands related to the space group Imma = \Gamma^0 D_{\text{26}}^{26} (74) with the Wannier functions being centered (a) at the La atoms, (b) at the Fe atoms, (c) at the As atoms, and (d) at the O atoms.

| \( \Gamma \)  | \( X \)  | \( R \)  | \( S \)  | \( T \)  | \( W \)  |
|------------|-------|-------|-------|-------|-------|
| Band 1     | \( 2\Gamma_{1}^+ + 2\Gamma_{3}^- \) | \( 2X_1^+ + 2X_3^- \) | \( 2R_1^+ + 2R_2^- \) | \( 2S_1^+ + 2S_3^- \) | T1 2W1 |
| Band 2     | \( 2\Gamma_{2}^+ + 2\Gamma_{4}^- \) | \( 2X_2^+ + 2X_4^- \) | \( 2R_1^+ + 2R_2^- \) | \( 2S_1^+ + 2S_3^- \) | T1 2W1 |
| Band 3     | \( 2\Gamma_{3}^+ + 2\Gamma_{1}^- \) | \( 2X_3^+ + 2X_1^- \) | \( 2R_1^+ + 2R_2^- \) | \( 2S_1^+ + 2S_3^- \) | T1 2W1 |
| Band 4     | \( 2\Gamma_{4}^+ + 2\Gamma_{2}^- \) | \( 2X_4^+ + 2X_2^- \) | \( 2R_1^+ + 2R_2^- \) | \( 2S_1^+ + 2S_3^- \) | T1 2W1 |

Notes to Table V:

(i) The antiferromagnetic structure of LaFeAsO depicted in Fig. 3(b) has the space group Imma and the magnetic group \( M = \text{Imma} + \{K\frac{1}{2} \frac{1}{2} 0\} \text{Imma} \) with \( K \) denoting the operator of time-inversion.

(ii) Each row defines one band consisting of four branches, because in each case there are four atoms in the unit cell.

(iii) The representations are given in Table II.

(iv) The bands are determined by Eq. (23) of Ref. 19.

(v) Assume a band of the symmetry in any row of these Tables V (a), (b), (c), or (d) to exist in the band structure of LaFeAsO. Then the Bloch functions of this band can be unitarily transformed into Wannier functions that are

- as well localized as possible;
- centered at the assigned (La, Fe, As, or O) atoms;
- and symmetry-adapted to the space group Imma.

(vi) Eq. (23) of Ref. 19 makes sure that the Wannier function may be chosen to be symmetry-adapted to the space group Imma. In addition, there exists a Matrix N satisfying both Eqs. (26) (with \( \{K\frac{1}{2} \frac{1}{2} 0\} \)) and (32) of Ref. 19 for all the bands listed in this table. Hence, the Wannier functions may be chosen symmetry adapted to the magnetic group \( M = \text{Imma} + \{K\frac{1}{2} \frac{1}{2} 0\} \text{Imma} \).