Structural Distortion in Antiferromagnetic BaFe$_2$As$_2$ as a Result of Time-Inversion Symmetry

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Abstract As reported by Q. Huang et al. (Phys. Rev. Lett. 101, 257003, 2008), neutron diffraction studies show an onset of antiferromagnetic order in BaFe$_2$As$_2$ associated with a tetragonal-to-orthorhombic distortion. We determine the group $\text{Cmca}$ as the space group of antiferromagnetic BaFe$_2$As$_2$ and identify a roughly half-filled energy band of BaFe$_2$As$_2$ with Bloch functions of special symmetry as magnetic band. As explained by the group-theoretical nonadiabatic Heisenberg model, the electrons in this narrow band may lower their Coulomb correlation energy by producing just the experimentally observed antiferromagnetic state if this state does not violate group-theoretical principles. However, in undistorted BaFe$_2$As$_2$ the time-inversion symmetry of the system interferes with the stability of the antiferromagnetic state. Nevertheless, it can be stabilized by a structural distortion of BaFe$_2$As$_2$ going beyond the magnetostriction. We derive two possible structural distortions stabilizing the antiferromagnetic state. These distortions are described by their space groups and consist in mere displacements of the Fe atoms.

Keywords Magnetism · Nonadiabatic Heisenberg model · Group theory

1 Introduction

Neutron diffraction investigations of BaFe$_2$As$_2$ [1] revealed a tetragonal-to-orthorhombic distortion associated with an antiferromagnetic order where the magnetic and the structural transitions occur at the same temperature. The present paper analyzes this obvious coincidence of magnetic and structural phase transitions in view of a group-theoretical approach which has already shed insight into the reasons for both magnetic and superconducting phases. This approach is based on the observation that the occurrence of a magnetic or superconducting state is always related to the existence of a narrow, almost half-filled magnetic or superconducting band of well-defined symmetry in the band structure of the respective material. Examples are the magnetic materials Cr [2], Fe [3], La$_2$CuO$_4$ [4], YBa$_2$Cu$_3$O$_6$ [5], and LaFeAsO [6], the (high-$T_c$) superconductors La$_2$CuO$_4$ [4], YBa$_2$Cu$_3$O$_7$, MgB$_2$ [7], and doped LaFeAsO [8], and numerous elemental superconductors [9, 10].

The notion of the used approach, the so-called nonadiabatic Heisenberg model, is that the electronic system in a narrow, roughly half-filled magnetic or superconducting band can lower its Coulomb correlation energy by condensing into an atomic-like state. However, for a consistent description of this atomic-like state we must also take into account the motion of the atomic cores following the electronic motion. Fortunately, we may assume that the very complex nonadiabatic localized functions representing the related localized states have the same symmetry and spin-dependence as the best localized, symmetry-adapted and, in the case of a superconducting band, spin-dependent Wannier functions of the magnetic or superconducting band. As a consequence of the special symmetry and spin-dependence of the localized states of a magnetic or superconducting band, the system is necessarily magnetic or a superconductor, respectively, in the atomic-like state [11]. In case of magnetic bands, however, an irrefutable condition is that related magnetic state does not conflict with the time-inversion symmetry of the system.
In Sect. 2 we shall identify the group \( Cmca (64) \) as the space group of the antiferromagnetic structure observed in Ba\( \text{Fe}_2\text{As}_2 \) (the number in parentheses is the international number) and shall determine the magnetic group of this structure. In the following Sect. 3 we will verify the existence of a magnetic band related to the observed antiferromagnetic structure in the band structure of Ba\( \text{Fe}_2\text{As}_2 \).

In Sect. 4 we shall show that this antiferromagnetic state is in fact unstable in undistorted Ba\( \text{Fe}_2\text{As}_2 \), because it conflicts with the time-inversion symmetry of the system. This statement means that the antiferromagnetic state exists in Ba\( \text{Fe}_2\text{As}_2 \) only, if it is accompanied by a distortion of the crystal going beyond the magnetostriction. Such distortions stabilizing an antiferromagnetic state have already been detected in La\( \text{CuO}_4 \) [4] and La\( \text{FeAsO} \) [6]. In Sect. 4.2 we will determine the space groups of those distortions for Ba\( \text{Fe}_2\text{As}_2 \) that stabilize the observed antiferromagnetic structure.

We shall find the two possible distortions (described by their space groups) depicted in Fig. 1, (c) and (d). Both distortions can be realized by a mere displacement of the iron atoms. We tend to the distortion in Fig. 1(c) to be most likely realized in Ba\( \text{Fe}_2\text{As}_2 \) because it clearly confirms the experimental observation by Huang et al. [1] that the \( a \) and \( b \) axes (denoted here in Fig. 1(b) by \( a_H \) and \( b_H \), respectively) have different lengths in the antiferromagnetic phase. Furthermore, this distortion is realized by nearest-neighbor Fe atoms that are oppositely displaced. Thus, the displacements are effected by a nearest-neighbor interaction between the Fe atoms which may be more efficient than an interaction between the Fe atoms in different layers as it appears to be effective in Fig. 1(d).

The nonadiabatic Heisenberg model does not distinguished between orbital and spin moments. Therefore, we always speak of “magnetic moments” which may consist of both orbital and spin moments.

2 The Magnetic Group of the Experimentally Observed Magnetic Structure

Figure 1(a) shows the two Fe atoms in the paramagnetic and Fig. 1(b) the four Fe atoms in the antiferromagnetic unit cell of Ba\( \text{Fe}_2\text{As}_2 \). By inspection we may recognize that Fig. 1(b) displays the experimentally determined [1] antiferromagnetic structure because by application of the given basic translations \( T_1, T_2, T_3 \) to the four Fe atoms in the unit cell we obtain just the magnetic structure presented in Fig. 3 of Ref. [1].

Removing from the space group \( I4/mmm \) of Ba\( \text{Fe}_2\text{As}_2 \) all the symmetry operations not leaving invariant the magnetic moments of the Fe atoms [as depicted in Fig. 1(b)], we obtain the group \( Cmca = \Gamma_0^b D_{2h}^{18} \) (64) as the space group of the antiferromagnetic structure in undistorted Ba\( \text{Fe}_2\text{As}_2 \). This may be proved using Fig. 1, (a) and (b), and also the “generating elements”

\[
\{ C_{2h}^1 | \frac{1}{2} \frac{1}{2} \frac{1}{2} \}, \quad \{ C_{2h}^2 | \frac{1}{2} \frac{1}{2} \frac{1}{2} \}, \quad \text{and} \quad \{ I | 0 0 0 \}
\]

of \( Cmca \), as it was detailed in Sect. 3.1 of Ref. [6]. The generating elements are taken from Table 5.7 of Ref. [6]; however, they are written in this paper in the coordinate system defined by Fig. 1(b), cf. the notes to Table 4.

Furthermore, by inspection of Fig. 1(b) we see that the antiferromagnetic structure in undistorted Ba\( \text{Fe}_2\text{As}_2 \) is invariant under the anti-unitary operation \( \{ K | \frac{3}{2} \frac{3}{2} \frac{3}{2} \} \), where \( K \) denotes the operator of time inversion reversing all the magnetic moments and leaving invariant the positions of the atoms. Thus, the magnetic group \( M_{64} \) of the experimentally determined magnetic structure in undistorted Ba\( \text{Fe}_2\text{As}_2 \) may be written as

\[
M_{64} = Cmca + [ K | \frac{3}{2} \frac{3}{2} \frac{3}{2} ] Cmca.
\]

3 Magnetic Band of Ba\( \text{Fe}_2\text{As}_2 \)

In this section we show that in the band structure of paramagnetic Ba\( \text{Fe}_2\text{As}_2 \) we find a magnetic band [11] related to the magnetic group \( M_{64} \) determined in the preceding section.

The band structure of paramagnetic Ba\( \text{Fe}_2\text{As}_2 \) (with the space group \( I4/mmm \)) is depicted in Fig. 2. There are Bloch functions near the Fermi level characterized by the representations

\[
\Gamma_5^+, \Gamma_3^+, Z_5^-, Z_4^-; X_1^-, X_3^+, X_4^+, X_4^+; N_1^+, N_2^-.
\]

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

\[
\begin{align*}
\Gamma_5^+ & \rightarrow \Gamma_2^+ + \Gamma_3^+ \\
Z_5^- & \rightarrow Y_2^- + Y_3^- \\
Z_4^- & \rightarrow Y_3^- \\
X_1^- & \rightarrow \Gamma_4^- \\
X_3^+ & \rightarrow Y_4^+ \\
X_4^- & \rightarrow \Gamma_3^- \\
X_4^+ & \rightarrow Y_3^+ \\
N_1^+ & \rightarrow R_1^- + R_2^- \\
N_2^- & \rightarrow R_1^+ + R_2^+ 
\end{align*}
\]

(see Table 5). The underlined representations form a magnetic band listed in Table 7, namely band 2. The representations \( Z_1 + Z_2 \) as well as \( T_1 + T_2 \) are absent in (4) though they belong to the magnetic band, too. They may be determined by the compatibility relations given in Tables 3 and 5.
The run of the magnetic band may not be visualized until the paramagnetic band structure is folded into the Brillouin zone of the antiferromagnetic structure lying diagonally within the Brillouin zone for the paramagnetic phase. Always two lines in the paramagnetic Brillouin zone are equivalent to one line in the antiferromagnetic Brillouin zone, see Table 1. The folded band structure with the magnetic band (highlighted by the bold line) is depicted in Fig. 3.

The Bloch functions of the magnetic band can be unitarily transformed into Wannier functions that are
- as well localized as possible,
- centered at the Fe atoms, and
- symmetry-adapted to the magnetic group $M_{64}$ in Eq. (2); see the notes to Table 7.

The magnetic band in BaFe$_2$As$_2$ is roughly half-filled and extremely narrow as compared with the other bands.
**Fig. 2** Band structure of tetragonal BaFe$_2$As$_2$ as calculated by the FHI-aims program [13, 14], using the structure parameters given in Ref. [1], with symmetry labels determined by the authors. The notation of the points and lines of symmetry in the Brillouin zone for $\Gamma_q^\pm$ follows Fig. 3.10 (b) of Ref. [12], and the symmetry labels are defined by Table 2.

**Fig. 3** The band structure of tetragonal BaFe$_2$As$_2$ (as given in Fig. 2) folded into the Brillouin zone for the Bravais lattice $\Gamma_q^{\pm}$ of the space group $Cmca$ of the antiferromagnetic structure. The bold line shows the magnetic band consisting of four branches with symmetry labels that can be identified from Table 4. The notation of the points and lines of symmetry follows Fig. 3.6(a) of Ref. [12]. The numbers labeling the branches at the line $\Delta$, $F$ characterize the related representations; for instance, the number 2 stands for $\Delta_2$ and $F_2$ (as defined in Table 6). In the surroundings of the sharp peaks at the line $\Delta$, $F$ (between $\Gamma$ and $\Gamma_{\pm}$), the Wannier functions are built from Bloch-like functions (Eq. (1.4) of Ref. [11]) of $\Delta_4$, $F_4$ symmetry that are linear combinations of two $\Delta_4$, $F_4$ Bloch functions arising from different lines in the Brillouin zone for the paramagnetic lattice $\Gamma_q^{\pm}$. These linear combinations smooth away the peaks. Similarly, the little jump between two $\Delta_2$ ($F_2$) branches near $Y_{\pm}$ is bridged by a linear combination of the related $\Delta_2$ ($F_2$) Bloch functions. Thus, this little jump is physically meaningless since it does not cross the Fermi level.
in the band structure of this material. Thus, this band provides optimal features enabling the electrons to lower their Coulomb correlation energy \([2, 3, 6, 11]\) by activating an exchange mechanism producing the experimentally determined antiferromagnetic structure. However, we shall show in the following section (Sect. 4) that in undistorted \(\text{BaFe}_2\text{As}_2\) this mechanism is blocked by the time-inversion symmetry of the system.

4 Stability of the Antiferromagnetic Structure

In this section we show that the antiferromagnetic state with the space group \(\text{Cmca}\) requires a (slight) distortion of \(\text{BaFe}_2\text{As}_2\) to form a different space group with restored time-inversion symmetry.

4.1 The Antiferromagnetic Structure is not Stable in Undistorted \(\text{BaFe}_2\text{As}_2\)

Assume that the magnetic state \(|G\rangle\) is an eigenstate of a Hamiltonian \(\hat{H}\) commuting with the operator \(K\) of time inversion,

\[
[\hat{H}, K] = 0, \tag{5}
\]
as it is the case within the nonadiabatic Heisenberg model, see Sect. III.C. of Ref. [2]. Nevertheless, we get a state different from \(|G\rangle\) when we apply \(K\) to \(|G\rangle\),

\[
K|G\rangle \neq |G\rangle, \tag{6}
\]
since \(K\) reverses the magnetic moments. Consequently [2], \(|G\rangle\) and \(K|G\rangle\) are basis functions of a two-dimensional irreducible corepresentations \(\tilde{D}\) of the magnetic group \(\tilde{M}\) of \(\hat{H}\). \(\tilde{M}\) may be written as

\[
\tilde{M} = M + KM, \tag{7}
\]
where \(M\) denotes the magnetic group

\[
M = S + \{K|t_K\}S \tag{8}
\]
of the magnetic state and \(S\) is the related space group.

However, when we restrict the symmetry operations to the subgroup \(M\) of \(\tilde{M}\), then \(\tilde{D}\) must subduce two onedimensional corepresentations \(D\) of \(M\), because, e.g., we have

\[
\{K|t_K\} |G\rangle = c \cdot |G\rangle, \tag{9}
\]
since the anti-unitary operator \(\{K|t_K\}\) belongs to the magnetic group \(M\) of the magnetic state; \(c\) is a complex number with \(|c| = 1\).

If the magnetic group \(\tilde{M}\) does not possess such suitable corepresentations \(\tilde{D}\), the related magnetic state is necessarily unstable. Fortunately, we may recognize by the known corepresentations of the space group \(S\) alone whether or not \(\tilde{M}\) possesses corepresentations \(\tilde{D}\) allowing a stable magnetic state. This may be carried out by means of Theorem 4.1 in Ref. [6] reading as follows:

**Theorem 1** The magnetic group \(\tilde{M}\) (7) possesses corepresentations allowing a stable magnetic state with the space group \(S\) if \(S\) has at least one one-dimensional single-valued representation

(i) following case (a) with respect to the magnetic group \(S + \{K|t_K\}S\) (8) of the magnetic state, and

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

The cases (a) and (c) are defined by Eqs. (7.3.45) and (7.3.47), respectively, of Ref. [12], and are given for the representations relevant in this paper in Tables 4, 8, and 9. This theorem led already to an understanding of the symmetry of the incommensurate spin-density-wave states in Cr [2].

At first sight, the representations at point \(R\) in the Brillouin for \(\text{Cmca}\) appear to comply with both conditions (i) and (ii), see Table 4. However, not all the space group operations of \(\text{Cmca}\) are comprised within the little group at \(R\), and, consequently, the magnetic group \(\tilde{M}\) (7) related to \(M = M_{64}\) (2) does not possess corepresentations allowing a stable antiferromagnetic state with the space group \(\text{Cmca}\).

4.2 Reaching Stability of the Antiferromagnetic State by Slight Distortion of the \(\text{BaFe}_2\text{As}_2\) Structure

The experimentally observed antiferromagnetic structure may be stabilized by a (small) distortion of the crystal that turns the space group \(\text{Cmca}\) into an “allowed” subgroup of \(\text{Cmca}\) possessing representations that allow the formation of a stable antiferromagnetic structure. In this context we considered all the space groups

(i) leaving invariant the experimentally observed magnetic structure depicted in Fig. 1(b), and

(ii) meeting the two conditions in Theorem 1.

In this way we found numerous allowed space groups in antiferromagnetic \(\text{BaFe}_2\text{As}_2\), among them also groups containing very few symmetry operations. In the following we only consider the space groups \(\text{Pnma}\) (62) and \(\text{Pbam}\) (55) which are the allowed space groups of highest symmetry in antiferromagnetic \(\text{BaFe}_2\text{As}_2\). Both groups have the orthorhombic-primitive Bravais lattice \(\Gamma_o\) and comprise the full orthorhombic point group \(D_{2h}\).
The space groups \( Pnma \) and \( Pbam \) can be defined by the generating elements
\[
\{ C_{2a}[01\frac{1}{2}] \}, \quad \{ C_{2z}[\frac{1}{2}0] \}, \quad \{ I[000] \}, \tag{10}
\]
and
\[
\{ C_{2a}[\frac{1}{2}0] \}, \quad \{ C_{2z}[000] \}, \quad \{ I[000] \}, \tag{11}
\]
respectively, as given in Table 3.7 of Ref. [12]. Here, however, they are written in the coordinate systems given by Fig. 1, (c) and (d), respectively.

The symmetry operations of both \( Pnma \) and \( Pbam \) leave invariant the atoms of \( \text{BaFe}_2\text{As}_2 \) and the antiferromagnetic structure depicted in Fig. 1(b). This may be proved starting from the generating elements of \( Pnma \) and \( Pbam \), as it was detailed in Sect. 5.1 of Ref. [6].

In contrast to the group \( Cmca \), both groups \( Pnma \) and \( Pbam \) possess one-dimensional representations satisfying both conditions (i) and (ii) of Theorem 1. These are the representations at point \( U \) in the Brillouin zone for \( Pnma \) and at points \( S \) and \( R \) in the Brillouin zone for \( Pbam \), see Tables 8 and 9, respectively. In any case, the little groups of the mentioned points \( U \), \( S \) and \( R \) comprise the whole space groups \( Pnma \) and \( Pbam \), respectively.

Consequently, an antiferromagnetic structure with the magnetic groups
\[
M_{62} = Pnma + \{ K[0\frac{1}{2}\frac{1}{2}] \} Pnma \tag{12}
\]
and
\[
M_{55} = Pbam + \{ K[0\frac{1}{2}\frac{1}{2}] \} Pbam \tag{13}
\]
can be stable in \( \text{BaFe}_2\text{As}_2 \).

These two magnetic groups \( M_{62} \) \( (12) \) and \( M_{55} \) \( (13) \) may be realized by the displacement of the Fe atoms as depicted in Fig. 1, (c) and (d). By means of the generating elements \( (10) \) and \( (11) \) we may verify that the symmetry operations of the space groups \( Pnma \) and \( Pbam \) leave these displacements of the Fe atoms invariant. In addition, the displacements of the Fe atoms are also invariant under the anti-unitary operations \( \{ K[0\frac{1}{2}\frac{1}{2}] \} \) and \( \{ K[\frac{1}{2}\frac{1}{2}0] \} \), respectively, since they connect in any case two atoms with antiparallel magnetic moments and the same displacement.

Consequently, the displacement of the Fe atoms depicted in Fig. 1, (c) and (d), stabilize the experimentally observed antiferromagnetic structure in \( \text{BaFe}_2\text{As}_2 \).

5 Summary

In Sects. 2 and 3 of this paper we could substantiate the existence of a magnetic band in the band structure of \( \text{BaFe}_2\text{As}_2 \) which is related to the magnetic group \( M_{64} \) \( (2) \) of the experimentally observed \( \text{[1]} \) antiferromagnetic state. As described by the nonadiabatic Heisenberg model, the electrons in this extremely narrow and roughly half-filled energy band can lower their Coulomb correlation energy by producing this antiferromagnetic state.

However, this lowering of the energy is forbidden in undistorted \( \text{BaFe}_2\text{As}_2 \) because a stable antiferromagnetic and its time-inverted state need to form a basis of a suitable irreducible corepresentation of the complete magnetic group of the Hamiltonian. Such a corepresentation is not available in an undistorted \( \text{BaFe}_2\text{As}_2 \) structure. However, as outlined in Sect. 4.2, a small shift of the Fe positions, brought about by the electron system in the magnetic band, makes the required corepresentation and thus a stable antiferromagnetic state.

We identified in Sect. 4 several distortions being able to stabilize the antiferromagnetic state in \( \text{BaFe}_2\text{As}_2 \). The two distortions with the highest symmetry are presented in Fig. 1, (c) and (d). They may be realized by the depicted small displacements of the Fe atoms which are invariant under the magnetic groups \( M_{62} \) \( (12) \) and \( M_{55} \) \( (13) \), respectively. The related space groups \( Pnma \) and \( Pbam \) have the same point group \( D_{2h} \) as \( Cmca \) but a lower translation symmetry; the translation \( T_1 \) in Fig. 1(b) is no longer a lattice translation in the distorted system, see Fig. 1, (c) and (d). We suppose that these two distortions of minor change of the symmetry are energetically more favorable than any other possible distortion of lower symmetry.

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Appendix: Group-Theoretical Tables

Table 1  Relationship between the lines of the Brillouin zones for the paramagnetic (Bravais lattice $\Gamma^b_q$) and the antiferromagnetic (Bravais lattice $\Gamma^b_p$) phases of undistorted BaFe$_2$As$_2$

\[
\begin{array}{cccccccccc}
\Delta_M \Gamma, \Delta_M X & \GammaZ, \GammaX, \GammaY, Z & \GammaM & \GammaO & \GammaO & \GammaO & \GammaO & \GammaO & \GammaO & \GammaO & \GammaO \\
\end{array}
\]

Notes
(i) Always two lines in the paramagnetic Brillouin zone are equivalent to one line in the antiferromagnetic Brillouin zone.
(ii) The space group $T_{mm}$ is isomorphic. Thus, the point group operations alone are symmetry operations.
(iii) The notation of the points and lines of symmetry follows Fig. 3.10(b) for $\Gamma^b_q$ and Fig. 3.6(a) for $\Gamma^b_p$ of Ref. [12].
(iv) XYUZ stands, e.g., for the line between X and Z via the lines Y and U in the Brillouin zone for BaFe$_2$As$_2$.
(v) $\Delta_M$ and $U_M$ stand for the central points of the lines $\Gamma \Delta_X$ and $XYUZ$, respectively, in the Brillouin zone for $\Gamma^b_q$.

Table 2  Character tables of the single-valued irreducible representations of the space group $I4/mmm = \Gamma^b_q D^{17}_{4d} (139)$ of tetragonal paramagnetic BaFe$_2$As$_2$

\[
\begin{array}{cccccccccc}
E & C_{2z} & C_{4z} & C_{2x} & C_{2y} & I & \sigma_z & S_{4x} & S_{4y} & \sigma_x & \sigma_{db} \\
\end{array}
\]

Note
(i) The space group $I4/mmm$ is symmorphic. Thus, the point group operations alone are symmetry operations.
(ii) The point group operations are related to the $x, y, z$ coordinates in Fig. 1(a).
(iii) The notation of the points of symmetry follows Fig. 3.10(b) of Ref. [12].
(iv) The character table is determined from Table 5.7 of Ref. [12].
Compatibility relations between points and lines in the Brillouin zone for tetragonal paramagnetic BaFe$_2$As$_2$ (space group $I4/mmm$)

| $\Gamma(000)$ | $X(00\frac{1}{2})$ |
|-------|-------|
| $\Gamma_1^+$ | $X_1^+$ |
| $\Gamma_2^+$ | $X_2^+$ |
| $\Gamma_3^+$ | $X_3^+$ |
| $\Gamma_4^+$ | $X_4^+$ |
| $\Gamma_1^-$ | $X_1^-$ |
| $\Gamma_2^-$ | $X_2^-$ |
| $\Gamma_3^-$ | $X_3^-$ |
| $\Gamma_4^-$ | $X_4^-$ |

$Z(\frac{1}{2} \frac{1}{2} \frac{1}{2})$

$Z_1^+ Z_2^+ Z_3^+ Z_4^+ Z_1^- Z_2^- Z_3^- Z_4^-$

$U_1 U_2 U_3 U_4 U_5 U_4 U_5 U_1 U_2$

Notes

(i) The notation of the points and lines of symmetry follows Fig. 3.10(b) of Ref. [12]

(ii) $Z(\frac{1}{2} \frac{1}{2} \frac{1}{2})$ and $X'(\frac{1}{2} \frac{1}{2} 0)$ are connected via the lines $U$ and $Y$. The symmetry labels are chosen in such a way that $U_i = Y_i$ (for $i = 1, 2, 3, 4$)

(iii) This table defines the labels $\Delta_i$ and $U_i$ which are needed in Table 5 to find the representations of the magnetic band at $Z$ and $T$

Character tables of the single-valued irreducible representations of the orthorhombic space group $Cmca = \Gamma_0^h D_{2h}^{18}$ (64) of the experimentally observed [1] antiferromagnetic structure depicted in Fig. 1(b)

$\Gamma(000)$ and $Y(\frac{1}{2} \frac{1}{2} 0)$

| $\Gamma(000)$ | $[E(000)]$ | $[C_{2h}^0 \frac{1}{2} \frac{1}{2} \frac{1}{2}]$ | $[C_{2h}^0 (000)]$ | $[I(000)]$ | $[\sigma_{db} \frac{1}{2} \frac{1}{2} \frac{1}{2}]$ | $[\sigma_{da} \frac{1}{2} \frac{1}{2} \frac{1}{2}]$ | $[\sigma_{dz} \frac{1}{2} \frac{1}{2} \frac{1}{2}]$ |
|-------|----------|----------|----------|--------|----------|----------|----------|
| $\Gamma_1^+$, $Y_1^+$ | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| $\Gamma_3^+$, $Y_3^+$ | 1 | -1 | 1 | -1 | 1 | -1 | 1 |
| $\Gamma_3^-$, $Y_3^-$ | 1 | 1 | -1 | -1 | 1 | 1 | -1 |
| $\Gamma_4^-$, $Y_4^-$ | 1 | -1 | -1 | 1 | 1 | 1 | -1 |

$Z(00\frac{1}{2})$ and $T(\frac{1}{2} \frac{1}{2} \frac{1}{2})$

| $\Gamma(000)$ | $[E(001)]$ | $[E(001)]$ | $[C_{2h}^0 \frac{1}{2} \frac{1}{2} \frac{1}{2}]$ | $[C_{2h}^0 \frac{1}{2} \frac{1}{2} \frac{1}{2}]$ | $[I(001)]$ | $[\sigma_{db} \frac{1}{2} \frac{1}{2} \frac{1}{2}]$ | $[\sigma_{da} \frac{1}{2} \frac{1}{2} \frac{1}{2}]$ | $[\sigma_{dz} \frac{1}{2} \frac{1}{2} \frac{1}{2}]$ |
|-------|----------|----------|----------|--------|--------|----------|----------|----------|
| $\Gamma_1^+$, $Y_1^+$ | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| $\Gamma_3^+$, $Y_3^+$ | 1 | -1 | 1 | -1 | 1 | -1 | 1 | 1 |
| $\Gamma_3^-$, $Y_3^-$ | 1 | 1 | -1 | -1 | 1 | 1 | -1 | 1 |
| $\Gamma_4^-$, $Y_4^-$ | 1 | -1 | -1 | 1 | 1 | 1 | -1 | 1 |

Notes

(i) The notation of the points of symmetry follows Fig. 3.6(a) of Ref. [12]

(ii) Point $S$ is not listed because it has only one two-dimensional representation $S_1$ irrelevant in this paper

(iii) The space group operations are related to the coordinate system in Fig. 1(b)

(iv) The character tables are determined from Table 5.7 in Ref. [12]. The origin of the coordinate system used in Ref. [12] for $Cmca$ is translated into the origin used in this paper by $T_0 = \frac{1}{4} T_1 + \frac{1}{4} T_2$. Thus, the symmetry operations $P_{hc}$ given in Table 5.7 of Ref. [12] are changed into the operations $P_h$ used in this paper by the equation $P_h = [E T_0] P_{hc} [E - T_0]$.

(v) The cases (a) and (c) are defined in Eqs. (7.3.45) and (7.3.47), respectively, of Ref. [12] and are determined by Eq. (7.3.51) of Ref. [12]
Table 5 Compatibility relations between the Brillouin zone for tetragonal paramagnetic BaFe$_2$As$_2$ and the Brillouin zone for the orthorhombic antiferromagnetic structure depicted in Fig. 1, (a) and (b), respectively

\[
\begin{array}{cccccccc}
\Gamma(000) & & & & X(00\frac{1}{2}) \\
\Gamma_1^+ & \Gamma_2^+ & \Gamma_3^+ & \Gamma_4^+ & \Gamma_5^- & \Gamma_6^- & \Gamma_1^- & \Gamma_2^- \\
\Gamma_1^+ & \Gamma_4^+ & \Gamma_1^+ & \Gamma_3^+ + \Gamma_3^- & \Gamma_1^- & \Gamma_2^- & \Gamma_1^- & \Gamma_2^- + \Gamma_3^- \\
& Z(\frac{1}{2} \frac{1}{2} \frac{1}{2}) & & & & & & \\
Z_1^+ & Z_2^+ & Z_3^+ & Z_4^+ & Z_5^- & Z_6^- & Z_1^- & Z_2^- \\
Y_4^+ & Y_3^+ & Y_4^+ & Y_2^+ + Y_3^+ & Y_1^- & Y_2^- & Y_3^- + Y_4^- \\
& N'(\frac{1}{2} \frac{1}{2} \frac{1}{2}) & & & & & & \\
N_1^+ & N_2^- & N_3^- & N_2^+ & N_2^- & N_2^- & N_2^- & N_2^- \\
R_1^+ + R_2^- & R_1^+ + R_2^- & R_1^+ + R_2^- & R_1^+ + R_2^- & R_1^+ + R_2^- & R_1^+ + R_2^- & R_1^+ + R_2^- & R_1^+ + R_2^- \\
& \Delta'_M(\frac{1}{2} \frac{1}{2} \frac{1}{2}) & & & & & & \\
\Delta_1 & \Delta_3 & \Delta_2 & \Delta_4 & \Delta_1 & \Delta_3 & \Delta_2 & \Delta_4 \\
& U'_M(\frac{1}{2} \frac{1}{2} \frac{1}{2}) & & & & & & \\
& U_1 & \tilde{U}_3 & \tilde{U}_2 & \tilde{U}_4 & U_1 & \tilde{U}_3 & \tilde{U}_2 & \tilde{U}_4 \\
\end{array}
\]

Notes

(i) The antiferromagnetic structure in Fig. 1(b) has the space group Cmca
(ii) The Brillouin zone for the orthorhombic space group Cmca lies within the Brillouin zone for the tetragonal space group I4/mmm
(iii) \(\Delta_M(00\frac{1}{2})\) and \(U_M(\frac{1}{2} \frac{1}{2} \frac{1}{2})\) stand for the central points of the lines connecting \(\Gamma\) with \(X(00\frac{1}{2})\) and \(Z(\frac{1}{2} \frac{1}{2} \frac{1}{2})\) with \(X'(\frac{1}{2} \frac{1}{2} \frac{1}{2})\), respectively
(iv) The points \(X', N', \Delta'_M, \) and \(U'_M\) do not belong to the basic domain of the Brillouin zone but can be generated by the action of the point group operations \(C_{4z}, C_{2z}, C_{4z},\) and \(C_{2z}\) on \(X, N, \Delta_M,\) and \(U_M,\) respectively
(v) 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 \(D_i\)
(vi) The symmetry labels for the points of symmetry are given in Tables 2 and 4, respectively
(vii) The symmetry labels for the lines \(\Delta\) and \(U\) are defined by Table 3
(viii) The compatibility relations are determined in the way described in great detail in Ref. [15]

Table 6 Compatibility relations between the points \(\Gamma(000)\) and \(Y(\frac{1}{2} \frac{1}{2} \frac{1}{2})\) and the line connecting these points in the Brillouin zone for the antiferromagnetic structure in undistorted BaFe$_2$As$_2$ (space group Cmca)

\[
\begin{array}{cccccccc}
\Gamma(000) & & & & Y(\frac{1}{2} \frac{1}{2} \frac{1}{2}) \\
\Gamma_1^+ & \Gamma_2^+ & \Gamma_3^+ & \Gamma_4^+ & \Gamma_1^- & \Gamma_2^- & \Gamma_1^- & \Gamma_2^- \\
\Delta_1 & \Delta_3 & \Delta_4 & \Delta_2 & \Delta_3 & \Delta_4 & \Delta_1 & \Delta_2 & \Delta_4 \\
& Y_1^+ & Y_2^+ & Y_3^+ & Y_4^+ & Y_1^- & Y_2^- & Y_3^- & Y_4^- \\
& F_1 & F_3 & F_4 & F_2 & F_1 & F_2 & F_4 \\
\end{array}
\]

Notes

(i) The notation of the points and lines of symmetry follows Fig. 3.6(a) of Ref. [12]
(ii) \(\Gamma(000)\) and \(Y(\frac{1}{2} \frac{1}{2} \frac{1}{2})\) are connected via the lines \(\Delta\) and \(F\). The symmetry notation is chosen in such a way that \(\Delta_i = F_i\) (for \(i = 1, 2, 3, 4\))
(iii) This table defines the labels \(\Delta_i\) and \(F_i\) which are needed to construct the magnetic band between \(\Gamma(000)\) and \(Y(\frac{1}{2} \frac{1}{2} \frac{1}{2})\) in Fig. 3
Table 7  Single-valued representations of all the energy bands of antiferromagnetic BaFe$_2$As$_2$ with symmetry-adapted and optimally localized Wannier functions centered at the Fe atoms

|       | $\Gamma$ | $Y$ | $Z$ | $T$ | $R$ |
|-------|-----------|-----|-----|-----|-----|
| Band 1 | $\Gamma_1^+ + \Gamma_2^+ + \Gamma_1^- + \Gamma_2^-$ | $Y_1^+ + Y_2^+ + Y_1^- + Y_2^-$ | $Z_1 + Z_2$ | $T_1 + T_2$ | $R_1^+ + R_2^+ + R_1^- + R_2^-$ |
| Band 2 | $\Gamma_3^+ + \Gamma_4^+ + \Gamma_3^- + \Gamma_4^-$ | $Y_1^+ + Y_2^+ + Y_1^- + Y_2^-$ | $Z_1 + Z_2$ | $T_1 + T_2$ | $R_1^+ + R_2^+ + R_1^- + R_2^-$ |

Notes
(i) The antiferromagnetic structure of undistorted BaFe$_2$As$_2$ depicted in Fig. 1(b) has the space group $Cmca$ and the magnetic group $M = Cmca + \{K|\frac{1}{2} \frac{1}{2} \frac{1}{2}\}Cmca$ with $K$ denoting the operator of time-inversion.
(ii) The two listed bands form “magnetic bands” related to $M$.
(iii) Each row defines one band consisting of four branches, because there are four Fe atoms in the unit cell.
(iv) The representations are given in Table 4.
(v) The bands are determined by Eq. (23) of Ref. [4].
(vi) Assume the tetragonal band structure of BaFe$_2$As$_2$ to be folded into the Brillouin zone for the antiferromagnetic phase (as carried out in Fig. 3) and assume further a band of the symmetry in any row of this table to exist in the folded band structure. Then the Bloch functions of this band can be unitarily transformed into Wannier functions that are

- as well localized as possible;
- centered at the Fe atoms; and
- symmetry-adapted to the space group $Cmca$ of the antiferromagnetic phase.

(vii) Equation (23) of Ref. [4] makes sure that the Wannier function may be chosen to be symmetry-adapted to the $space$ group $Cmca$ of the antiferromagnetic phase. In addition, there exists a matrix $N$, namely

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

satisfying both Eqs. (26) (with $\{K|\frac{1}{2} \frac{1}{2} \frac{1}{2}\}$) and (32) of Ref. [4] for the two bands listed in this table. Hence, the Wannier functions may be chosen symmetry-adapted to the magnetic group $M = Cmca + \{K|\frac{1}{2} \frac{1}{2} \frac{1}{2}\}Cmca$.

Table 8  Character table of the single-valued irreducible representations of the orthorhombic space group $Pnma = \Gamma_s D_{2h}^{16}$ (62)

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

|       | $\{K|\frac{1}{2} \frac{1}{2} \frac{1}{2}\}$ | $\{E|000\}$ | $\{C_{2\alpha}|0 \frac{1}{2} \frac{1}{2}\}$ | $\{E|001\}$ | $\{C_{2\alpha}|0 \frac{1}{2} \frac{1}{2}\}$ | $\{C_{2\beta}|\frac{1}{2} \frac{1}{2} \frac{1}{2}\}$ | $\{C_{2\beta}|\frac{1}{2} \frac{1}{2} \frac{1}{2}\}$ |
|-------|---------------------------------|-------------|---------------------------------|-------------|---------------------------------|---------------------------------|---------------------------------|
| $U_1^-$ (c) (a) | 1 | i | -1 | -i | 1 | i | -1 |
| $U_2^-$ (c) (a) | 1 | -i | -1 | i | 1 | -i | -1 |
| $U_3^-$ (c) (a) | 1 | i | -1 | -i | -1 | -i | 1 |
| $U_4^-$ (c) (a) | 1 | -i | -1 | i | -1 | i | 1 |
| $U_1^+$ (c) (a) | 1 | i | -1 | -i | 1 | i | -1 |
| $U_2^+$ (c) (a) | 1 | -i | -1 | i | 1 | -i | -1 |
| $U_3^+$ (c) (a) | 1 | i | -1 | -i | -1 | -i | 1 |
| $U_4^+$ (c) (a) | 1 | -i | -1 | i | -1 | i | 1 |
### Table 8 (Continued)

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

| $\left. \chi \right| \frac{1}{2} \frac{1}{2} \frac{1}{2}$ | $\left. \chi \right| \frac{1}{2} \frac{1}{2} 0$ | $\left. \chi \right| \frac{1}{2} \frac{1}{2} 1$ | $\left. \chi \right| \frac{1}{2} \frac{1}{2} \frac{1}{2}$ | $\left. \chi \right| \frac{1}{2} \frac{1}{2} \frac{1}{2}$ | $\left. \chi \right| \frac{1}{2} \frac{1}{2} \frac{1}{2}$ | $\left. \chi \right| \frac{1}{2} \frac{1}{2} \frac{1}{2}$ |
|---|---|---|---|---|---|---|
| $U_1^-$ | -i | 1 | i | -1 | i | 1 | -1 | -i |
| $U_2^+$ | i | 1 | -i | -1 | i | 1 | -1 | i |
| $U_3^-$ | i | 1 | -1 | -i | i | 1 | -1 | -i |
| $U_4^-$ | -i | 1 | -i | -1 | i | 1 | -1 | i |
| $U_1^+$ | -i | -1 | i | 1 | -1 | -i | -i |
| $U_2^+$ | i | -1 | i | 1 | -1 | -i | i |
| $U_3^+$ | i | -1 | i | 1 | -1 | -i | -i |
| $U_4^+$ | -i | -1 | i | 1 | -1 | -i | i |

Notes:
(i) The notation of the points of symmetry follows Fig. 3.5 of Ref. [12]
(ii) Only the listed point $U$ is relevant in this paper
(iii) The notation of the space group operations is related to the coordinate system in Fig. 1(c)
(iv) The character table is determined from Table 5.7 in Ref. [12]. The origin of the coordinate system used in Ref. [12] for $Pnma$ is identical with the origin used in this paper
(v) The cases (a) and (c) are defined in Eqs. (7.3.45) and (7.3.47), respectively, of Ref. [12] and are determined by Eq. (7.3.51) of Ref. [12]

### Table 9

Character tables of the single-valued irreducible representations of the orthorhombic space group $Pbam = \Gamma_oD_{2h}^9$ (55)

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

| $K$ | $\left. \chi \right| \frac{1}{2} \frac{1}{2} 0$ | $\left. \chi \right| \frac{1}{2} \frac{1}{2} 0$ | $\left. \chi \right| \frac{1}{2} \frac{1}{2} 0$ | $\left. \chi \right| \frac{1}{2} \frac{1}{2} 0$ | $\left. \chi \right| \frac{1}{2} \frac{1}{2} 0$ | $\left. \chi \right| \frac{1}{2} \frac{1}{2} 0$ |
|---|---|---|---|---|---|---|
| $S_{1}^-$ | (c) | (a) | 1 | i | -1 | i | 1 | -1 |
| $S_{2}^+$ | (c) | (a) | 1 | -i | -1 | i | 1 | -1 |
| $S_{3}^+$ | (c) | (a) | 1 | i | -1 | -i | 1 | -i |
| $S_{4}^+$ | (c) | (a) | 1 | -i | -1 | i | 1 | -1 |
| $S_{1}^+$ | (c) | (a) | 1 | i | -1 | -i | 1 | -i |
| $S_{2}^+$ | (c) | (a) | 1 | -i | -1 | i | 1 | -1 |
| $S_{3}^+$ | (c) | (a) | 1 | i | -1 | -i | 1 | -i |
| $S_{4}^+$ | (c) | (a) | 1 | -i | -1 | i | 1 | -1 |

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

| $\left. \chi \right| \frac{1}{2} \frac{1}{2} 0$ | $\left. \chi \right| \frac{1}{2} \frac{1}{2} 0$ | $\left. \chi \right| \frac{1}{2} \frac{1}{2} 0$ | $\left. \chi \right| \frac{1}{2} \frac{1}{2} 0$ | $\left. \chi \right| \frac{1}{2} \frac{1}{2} 0$ | $\left. \chi \right| \frac{1}{2} \frac{1}{2} 0$ | $\left. \chi \right| \frac{1}{2} \frac{1}{2} 0$ |
|---|---|---|---|---|---|---|
| $S_{1}^-$ | -i | 1 | i | -1 | -i | 1 | i |
| $S_{2}^+$ | i | 1 | -i | -1 | i | 1 | -1 |
| $S_{3}^+$ | i | 1 | -1 | -i | i | 1 | -1 |
| $S_{4}^+$ | -i | 1 | -1 | -i | i | 1 | -1 |
| $S_{1}^+$ | -i | -1 | i | 1 | -1 | -i | 1 |
| $S_{2}^+$ | i | -1 | i | 1 | -1 | -i | i |
| $S_{3}^+$ | i | -1 | i | 1 | -1 | -i | -i |
| $S_{4}^+$ | -i | -1 | i | 1 | -1 | -i | i |
Table 9 (Continued)

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

| \(K\) | \(\{K\} [\frac{1}{2} \frac{1}{2} 0]\) | \(\{E\} [0 0 0]\) | \(\{C_{2h}\} [\frac{1}{2} \frac{1}{2} 0]\) | \(\{E\} [0 0 1]\) | \(\{C_{2h}\} [\frac{1}{2} \frac{1}{2} 1]\) | \(\{C_{2h}\} [0 0 0]\) | \(\{C_{2h}\} [\frac{1}{2} \frac{1}{2} 0]\) | \(\{C_{2h}\} [0 0 1]\) |
|-----|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| \(R_1\) | \(\{c\}\) (a) | 1 | \(i\) | \(-1\) | \(-i\) | 1 | \(i\) | \(-1\) |
| \(R_2\) | \(\{c\}\) (a) | 1 | \(-i\) | \(-1\) | \(i\) | 1 | \(-i\) | \(-1\) |
| \(R_3\) | \(\{c\}\) (a) | 1 | \(i\) | \(-1\) | \(-i\) | 1 | \(-i\) | \(-1\) |
| \(R_4\) | \(\{c\}\) (a) | 1 | \(-i\) | \(-1\) | \(i\) | 1 | \(-1\) | \(-1\) |
| \(R_5\) | \(\{c\}\) (a) | 1 | \(i\) | \(-1\) | \(-i\) | 1 | \(i\) | \(-1\) |
| \(R_6\) | \(\{c\}\) (a) | 1 | \(-i\) | \(-1\) | \(i\) | 1 | \(-1\) | \(-1\) |
| \(R_7\) | \(\{c\}\) (a) | 1 | \(i\) | \(-1\) | \(-i\) | 1 | \(-i\) | \(-1\) |
| \(R_8\) | \(\{c\}\) (a) | 1 | \(-i\) | \(-1\) | \(i\) | 1 | \(-1\) | \(-1\) |

Notes

(i) The notation of the points of symmetry follows Fig. 3.5 of Ref. [12]
(ii) Only the listed points \(S\) and \(R\) are relevant in this paper
(iii) The notation of the space group operations is related to the coordinate system in Fig. 1(d)
(iv) The character tables are determined from Table 5.7 in Ref. [12]. The origin of the coordinate system used in Ref. [12] for \(Pbam\) is identical with the origin used in this paper
(v) The cases (a) and (c) are defined in Eqs. (7.3.45) and (7.3.47), respectively, of Ref. [12] and are determined by Eq. (7.3.51) of Ref. [12]

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