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FERROMAGNETISM IN QUASICRYSTALS: SYMMETRY ASPECTS

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Magnetic-group analysis of the symmetries typical of quasicrystals shows that ferromagnetism is incompatible with the icosahedral symmetry. Depending on the magnetic field direction, the icosahedral symmetry in the magnetic field is reduced to pentagonal, trigonal or rhombic symmetries.

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Quasicrystals are currently attracting great interest for the variety of their unusual physical properties. Among these, the magnetic properties, and especially ferromagnetism are the least studied. The first experimental information on ferromagnetism in quasicrystals was connected with the presence of ferromagnetic non-quasicrystalline inclusions of a second phase [1, 2], and later ferromagnetic-like behavior was observed in pure icosahedral phases *i*-AlPdMnB and *i*-AlPdFeB [3, 4]. Mössbauer spectroscopy and nuclear magnetic resonance (NMR) experiments have shown that the magnetic state in these systems was ferromagnetic, but the samples consisted of large magnetic clusters with extensions of about 20 nm [2, 4]. Theoretically, the ferromagnetic ordering in quasicrystals has never been considered, and the most important problem is the compatibility of ferromagnetism with quasicrystalline symmetries. To the best of our knowledge, it has never been considered before, although the color groups for quasicrystalline solids have been studied [5, 6]. In the present work, a theoretical analysis of the magnetic groups for quasicrystals is performed to solve this problem.

The existence of a magnetic structure in solids is formally connected with the time inversion operation. The time inversion symmetry operation R changes the direction of the current density in a solid but does not act on spatial coordinates. The element R commutes with the rotations C_n, the rotations S_{2n}, and the reflections σ, and at the same time, $R^2 = E$ (the identity transformation). Magnetic crystalline classes for periodic solids are described in Ref. [7]. Structurally, magnetic classes can be divided into three types. The magnetic class of type I has the ordinary point group symmetry. The direct product of point groups with the group $\{E, R\}$ forms the magnetic class of type II. The magnetic class of type III contains the operation R in combination with some rotations or reflections. These magnetic classes have the structure $\mathbf{G(H)}=\mathbf{H}+\mathbf{R}g\mathbf{H}$, where $\mathbf{H}$ is an invariant subgroup of index 2, $g \in \mathbf{G}$, but $g \notin \mathbf{H}$, and $\mathbf{R}$ is the time inversion operator. In periodic solids, 58 magnetic classes of type III exist. In this paper, we obtain the magnetic classes for quasiperiodic structures following the method described in Ref. [7]

We first obtain the magnetic classes for symmetries with a preferable main axis (we have the 5-fold, 8-fold, 10-fold, and 12-fold axes in mind). Classes with such a symmetry are related to pentagonal, octagonal, decagonal, and dodecagonal systems, correspondingly. The magnetic classes of type I represent an ordinary point group. Ferromagnetism is possible in the following classes of type I: $\boldsymbol{C}_5$, $\boldsymbol{C}_{5h}$, $\boldsymbol{C}_8$, $\boldsymbol{C}_{8h}$, $\boldsymbol{S}_8$, $\boldsymbol{C}_{10}$, $\boldsymbol{C}_{10h}$,

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Magnetic classes for quasicrystalline symmetries

Symmetry	Point groups	Magnetic classes of type III	Ferromagnetic classes
Pentagonal	$\boldsymbol{C}_5, \boldsymbol{C}_{5v}, \boldsymbol{D}_5, \boldsymbol{S}_{10}, \boldsymbol{D}_{5d}$	$\boldsymbol{C}_{5v}(\boldsymbol{C}_5)$, $\boldsymbol{D}_5(\boldsymbol{C}_5)$, $\boldsymbol{S}_{10}$ $(\boldsymbol{C}_5)$, $\boldsymbol{D}_{5d}$ $(\boldsymbol{C}_{5v}, \boldsymbol{D}_5, \boldsymbol{S}_{10})$	$\boldsymbol{C}_{5v}$ $(\boldsymbol{C}_5)$, $\boldsymbol{D}_5$ $(\boldsymbol{C}_5)$, $\boldsymbol{D}_{5d}$ $(\boldsymbol{S}_{10})$
Octagonal	$\boldsymbol{C}_8, \boldsymbol{S}_8, \boldsymbol{C}_{8v}, \boldsymbol{D}_8, \boldsymbol{C}_{8h}, \boldsymbol{D}_{4d}, \boldsymbol{D}_{8h}$	$\boldsymbol{C}_8$ $(\boldsymbol{C}_4)$, $\boldsymbol{S}_8$ $(\boldsymbol{C}_4)$, $\boldsymbol{C}_{8v}$ $(\boldsymbol{C}_8, \boldsymbol{C}_{4v})$, $\boldsymbol{D}_8$ $(\boldsymbol{C}_8, \boldsymbol{D}_4)$, $\boldsymbol{C}_{8h}$ $(\boldsymbol{C}_8, \boldsymbol{C}_{4h}, \boldsymbol{S}_8)$, $\boldsymbol{D}_{4d}$ $(\boldsymbol{D}_4, \boldsymbol{C}_{4v}, \boldsymbol{S}_8)$, $\boldsymbol{D}_{8h}$ $(\boldsymbol{C}_{8h}, \boldsymbol{C}_{8v}, \boldsymbol{D}_8, \boldsymbol{D}_{4h}, \boldsymbol{D}_{4d})$	$\boldsymbol{C}_{8v}$ $(\boldsymbol{C}_8)$, $\boldsymbol{D}_8$ $(\boldsymbol{C}_8)$, $\boldsymbol{D}_{4d}$ $(\boldsymbol{S}_8)$, $\boldsymbol{D}_{8h}$ $(\boldsymbol{C}_{8h})$
Decagonal	$\boldsymbol{C}_{10}, \boldsymbol{C}_{5h}, \boldsymbol{C}_{10v}, \boldsymbol{D}_{10}, \boldsymbol{C}_{10h}, \boldsymbol{D}_{5h}, \boldsymbol{D}_{10h}$	$\boldsymbol{C}_{10}$ $(\boldsymbol{C}_5)$, $\boldsymbol{C}_{5h}$ $(\boldsymbol{C}_5)$, $\boldsymbol{C}_{10v}$ $(\boldsymbol{C}_{10}, \boldsymbol{C}_{5v})$, $\boldsymbol{D}_{10}$ $(\boldsymbol{C}_{10}, \boldsymbol{D}_5)$, $\boldsymbol{C}_{10h}$ $(\boldsymbol{C}_{10}, \boldsymbol{C}_{5h}, \boldsymbol{S}_{10})$, $\boldsymbol{D}_{5h}$ $(\boldsymbol{D}_5, \boldsymbol{C}_{5v}, \boldsymbol{C}_{5h})$, $\boldsymbol{D}_{10h}$ $(\boldsymbol{C}_{10h}, \boldsymbol{C}_{10v}, \boldsymbol{D}_{10}, \boldsymbol{D}_{5h}, \boldsymbol{D}_{5d})$	$\boldsymbol{C}_{10v}$ $(\boldsymbol{C}_{10})$, $\boldsymbol{D}_{10}$ $(\boldsymbol{C}_{10})$, $\boldsymbol{D}_{5h}$ $(\boldsymbol{C}_{5h})$, $\boldsymbol{D}_{10h}$ $(\boldsymbol{C}_{10h})$
Dodecagonal	$\boldsymbol{C}_{12}, \boldsymbol{S}_{12}, \boldsymbol{C}_{12v}, \boldsymbol{D}_{12}, \boldsymbol{C}_{12h}, \boldsymbol{D}_{6d}, \boldsymbol{D}_{12h}$	$\boldsymbol{C}_{12}$ $(\boldsymbol{C}_6)$, $\boldsymbol{S}_{12}$ $(\boldsymbol{C}_6)$, $\boldsymbol{C}_{12v}$ $(\boldsymbol{C}_{12}, \boldsymbol{C}_{6v})$, $\boldsymbol{D}_{12}$ $(\boldsymbol{C}_{12}, \boldsymbol{D}_6)$, $\boldsymbol{C}_{12h}$ $(\boldsymbol{C}_{12}, \boldsymbol{C}_{6h}, \boldsymbol{S}_{12})$, $\boldsymbol{D}_{6d}$ $(\boldsymbol{D}_6, \boldsymbol{C}_{6v}, \boldsymbol{S}_{12})$, $\boldsymbol{D}_{12h}$ $(\boldsymbol{C}_{12h}, \boldsymbol{C}_{12v}, \boldsymbol{D}_{12}, \boldsymbol{D}_{6h}, \boldsymbol{D}_{6d})$	$\boldsymbol{C}_{12v}$ $(\boldsymbol{C}_{12})$, $\boldsymbol{D}_{12}$ $(\boldsymbol{C}_{12})$, $\boldsymbol{D}_{6d}$ $(\boldsymbol{S}_{12})$, $\boldsymbol{D}_{12h}$ $(\boldsymbol{C}_{12h})$
Icosahedral	$\boldsymbol{Y}, \boldsymbol{Y}_h$	$\boldsymbol{Y}_h(\boldsymbol{Y})$	–

$\boldsymbol{S}_{10}$, $\boldsymbol{C}_{12}$, $\boldsymbol{C}_{12h}$, and $\boldsymbol{S}_{12}$, with the magnetic moment vector directed along the main axis. Of course, ferromagnetism is impossible in all type-II magnetic classes (due to the presence of the time inversion R).

As pointed out above, all possible index-2 subgroups should be determined in order to find the magnetic classes of type III. The simplest way is to use the tables of characters of irreducible representations. Classes with characters equal to one in one-dimensional representations form invariant subgroups of index 2. All possible groups are given in the Table for the systems under consideration. Each magnetic class is defined by a point group and its index-2 subgroup (in parentheses), which is given in the Table. We note that only the class C_5 does not have index-2 subgroups, and consistently magnetic classes of type III. For the existence of the ferromagnetic state in magnetic classes of type III, it is necessary that these classes do not contain the elements RI or R_{σ_h} (I is the spatial inversion and σ_h is the reflection in the plane perpendicular to the main axis). All classes of type III that allow a ferromagnetic state are given in the last column in the Table. The magnetic moment vector in these classes is directed along the main axis.

In the case of the icosahedral symmetry, there is only one class $\boldsymbol{Y}_h$ $(\boldsymbol{Y})$ of type III. In this class, it is impossible (due to the presence of the operation RI) to find a direction for which the magnetic moment vector is invariant under all symmetry operations. But due to different conditions (magnetostriction, external field, etc.), the icosahedral symmetry (the groups $\boldsymbol{Y}$ and $\boldsymbol{Y}_h$) can be reduced to the pentagonal groups $\boldsymbol{D}_5$ and $\boldsymbol{D}_{5d}$ if the action is along one of the 5-fold axes or to the trigonal ($\boldsymbol{D}_3$ and $\boldsymbol{D}_{3d}$) and rhombic ($\boldsymbol{D}_2$ and $\boldsymbol{D}_{2h}$) groups if the action is along one of the 3-fold or 2-fold axes. In this sense, the possibility of ferromagnetism in icosahedral quasicrystals is analogous to the ferromagnetism in crystals with the cubic symmetry. It is known that the lattice of the ferromagnetic phase of iron is not cubic (body-centered cubic) but tetragonal with the tetragonal distortion of the order 10^{-5} [7, 8], which is too small to be observed experimentally. A distortion of the icosahedral quasicrystal (with the group $\boldsymbol{Y}_h$) due to magnetostriction along one of the 5-order axes should reduce the symmetry to the class $\boldsymbol{D}_{5d}$, which forms the ferromagnetic class $\boldsymbol{D}_{5d}$ $(\boldsymbol{S}_{10})$.

In quasicrystals, magnetostriction can generate phasons, and as a result a sample becomes magnetically inhomogeneous. Actually, the experiments mentioned above have been explained in terms of large magnetic clusters with the size about 20 nm [2, 3]. Therefore, the magnetic state of these objects may be characterized as the «mictomagnetic» (mixed) one. For the mictomagnetic state, the susceptibility is analogous to an antiferromagnetic or spin glass state, but spontaneous magnetization after cooling in the field is typical of ferromagnets [8, 9]. In this sense, the «ferromagnetic» quasicrystals have many features in common with concentrated alloys CuMn and AuFe, where magnetic behavior can be described by the presence of large supermagnetic clusters with identical moments and anisotropy fields, but with random directions of the light magnetization axis. Upon increasing the concentration, creation of magnetic clusters becomes more probable and the long-range magnetic order can propagate over the entire sample [8, 9].

In conclusion, based on a magnetic-group analysis, we have predicted that ferromagnetism is incompatible with the icosahedral symmetry of quasicrystals. In a magnetic field, the icosahedral symmetry is reduced to the pentagonal or trigonal or rhombic symmetry depending on the field direction. Magnetostriction can induce phason distortions in quasicrystals, and as a result the system becomes magnetically inhomogeneous. Such a physical picture can explain the existing experimental data on «ferromagnetic» quasicrystals.

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