Symmetry of electron states in antiferromagnets

S. A. Brazovskiĭ and I. A. Luk'yanchuk

L. D. Landau Institute of Theoretical Physics, Academy of Sciences of the USSR
(Submitted 11 April 1989; resubmitted 6 June 1989)
Zh. Eksp. Teor. Fiz. **96**, 2088–2095 (December 1989)

The symmetry of the electron states in an antiferromagnetically ordered crystal is investigated. The elements of the two-value corepresentation apparatus for the magnetic groups are used in a form that corresponds to the models and methods of the microscopic theories. The symmetry restrictions on the quasiparticle spectra, on their interaction with the magnetic field **h**, and on the interband matrix elements are found. The spin-orbit effects are considered. It is shown that a field **h** perpendicular to the antiferromagnetic ordering vector **n** does not split the twofold degeneracy of the states at the boundary of the magnetic Brillouin zone but shifts the spectrum extrema away from the boundary. The results are illustrated for the case of a two-dimensional system corresponding to the CuO_2 plane in weakly doped high-temperature superconductors. The general conclusions are applicable to itinerant antiferromagnets, including quasi-one-dimensional compounds with a spin density wave.

1. INTRODUCTION

The observation[1,2] of an antiferromagnetic (AFM) phase in high-temperature superconducting (HTSC) materials stimulated theoretical study of the electronic states in magnetically ordered media long known as "magnetic semiconductors[3,4]" or "spin-density waves (SDW)."[5,6] Regardless of the success or difficulties of the microscopic models, based on weak- or strong-coupling approximations, it is feasible to carry out an analysis based purely on symmetry which can establish a set of model-independent results. A symmetry-based approach, and group theory methods, have always been basic tools in the theory of semiconductors, allowing determination of spectra, effective Hamiltonians, selection rules, etc.

In this study we apply symmetry methods to the description of electronic states in antiferromagnets in an insulating or weakly doped phase. Classification of states for various points of the Brillouin zone and a series of selection rules will be given, and the interaction of electrons with an external magnetic field or with their intrinsic magnetic moment will be examined. Effects accessible to direct experimental verification are found for the magnetic properties. Specific studies are carried out for an antiferromagnet on a quadratic lattice with point symmetry group D_4, for the CuO_2 layer in the HTSC compounds La_2CuO_4.

In the AFM-ordered phase the quantum numbers of charged quasi-particles, generally speaking, are indeterminate, since spin is not a conserved quantum number. None the less, a group-theoretical classification always applies: each elementary excitation manifests an irreducible representation λ of the full group symmetry of the system. These representations determine the Lehmann expansion (see Ref. 7) of the exact single-particle electron Green's function

$$G(\mathbf{r},\mathbf{r}')=\sum_{\lambda}\frac{\psi_\lambda(\mathbf{r})\psi_\lambda^*(\mathbf{r}')}{\varepsilon-\varepsilon_\lambda}.$$

In talking further about the wave functions ψ_λ in the spectra ε_λ, we will have in mind these values. The versions of the corresponding creation operators and single-particle Hamiltonians used further on are correct in the self-consistent-field approximation for weak-coupling nesting models (see the reviews of Refs. 4–6). In this model the spin projection on the AFM-ordering axis is a conserved quantity; this naturally corresponds to a two-value corepresentation (see Sec. 2), which is model-independent.

From a symmetry point of view the electronic spinor wave functions ψ_λ in an AFM are the basic functions of two-valued irreducible corepresentations of the symmetry group of the system, which contains anti-unitary elements: combinations of time-reversal operations R with spatial transformations. The formal theory and enumeration of all the corepresentations of the crystal groups are presented in Ref. 8. However, the abstraction and brevity of the exposition, due to the necessity for examining a large number of space groups, complicate their use in a multi-electron theory of magnetically-ordered states. In connection with present problems in the theory of band antiferromagnetism, it can be useful to have a treatment of the symmetry properties corresponding to the methods of the microscopic models. Therefore it is useful to discuss the way to find the two-value irreducible corepresentations of the crystal groups, which generalizes the construction of electronic Bloch functions in the normal metal, is natural from the physical point of view, and takes into account in a clear way the direction **n** of the AFM order parameter in the crystal (Sec. 2). We limit ourselves to the simplest case of a two-sublattice collinear AFM on a square lattice with D_4 symmetry, which corresponds to a CuO_2 layer in HTSC compounds of the La_2CuO_4 type. It is obvious that for complex magnetic groups a comprehensive symmetry analysis of the magnetic extrema, regardless of their origin, can be more efficiently done only on the basis of formal methods.[8] Up to the present the corresponding studies have not really been carried out.

2. THE SYMMETRY GROUP

A description of particles with spin, as a rule, has been based on the transformational properties of their wave functions (spinors) relative to time. Spinors are a two-value representation of the rotation group, from which their properties relative to time reversal R also come. An alternative approach originating from their transformation properties

 0038-5646/89/121180-05$04.00

relative to R is also possible. In this treatment the same wave functions are realizations of so-called two-value corepresentations.[8] In describing particles in a magnetically ordered medium, where the full group symmetry relative to rotation in spin space is destroyed, the second approach is more natural.

Let us examine first the symmetry group $\mathcal{G}$ belonging to a collinear two-sublattice antiferromagnet on the sites of a square lattice. In this part we will neglect the weak relativistic effects of spin-orbit interaction with the crystal lattice for both conduction electrons and ordered moments in comparison with the exchange interaction between electrons and moments (see Sec. 5 further on). In this approximation we assume that the position of spin space is not fixed relative to coordinate space; that is, all coordinate space rotations do not act on the electron spins.[9] Therefore, the system wave function is sensitive to the magnetic order of the antiferromagnet only for those group symmetry operations of the crystal which interchange the magnetic sublattices; that is, which are combined with the time reversal operation R. For the systems of interest to us, on a square lattice, only the translations T_x and T_y over the periods $\mathbf{a}_x$ and $\mathbf{a}_y$ of the lattice are such operations, if the center of coordinates is chosen to be one of its sites. The symmetry group of the antiferromagnet on the square lattice is $\mathcal{G}=\{D_4, RT_x, RT_y\}$.

We will be interested in the two-value irreducible representations (more accurately, corepresentations, as RT is an anti-unitary operator) of the group $\mathcal{G}$ corresponding to the electron wave function. The formal theory of corepresentations of crystal groups is presented in Ref. 8; however, the abstract exposition makes physical application difficult. In the following derivations we will find it useful to describe the derivation of the two-value representations of the group $\mathcal{G}$ with instructions on the physical meaning of the terms used.

The two-value representations of the group $\mathcal{G}$ are direct generalizations of the two-value irreducible representations of the space groups, calculation of which reduces, as we know,[10] to construction of the star $\{\mathbf{k}\}$ of the wave vector $\mathbf{k}$ and the derivation of the two-value irreducible representations of the symmetry group of this vector (the small group). The region in which the vector $\mathbf{k}$ is determined—the Brillouin zone—should be chosen so that any two basis functions corresponding to different vectors $\mathbf{k}$ do not transform identically under the action of $\mathcal{G}$. By analogy with the construction of representations of space groups we will consider that the two-value corepresentations of the small group of the vector $\mathbf{k}$ for the group $\mathcal{G}$ having a center of inversion are characterized by a two-component wave function $\varphi_{\mathbf{k}}=(u_{\mathbf{k}}, v_{\mathbf{k}})$. The operations $RT_i\,(i=x,y)$ entering into the makeup of the elements of $\mathcal{G}$, aside from acting on the components $u_{\mathbf{k}}$, $v_{\mathbf{k}}$, change the sign of $\mathbf{k}$. Therefore, it will be convenient for us to combine the spinors $\varphi_{\mathbf{k}}$ and $\varphi_{-\mathbf{k}}$ in a four-component function $(\varphi_{\mathbf{k}}, \varphi_{-\mathbf{k}})$.

Let us say that for the operators RT_i the spinor $\varphi_{\mathbf{k}}$ transforms under the action of the matrices $\hat{U}_i$. In determining $\hat{U}_i$ we consider first the group $\mathcal{F}=\{D_4, (RT_x)^2, (RT_y)^2\}$; $\mathcal{F}\subset\mathcal{G}$. Then we expect that the matrix corresponding to the operation $(RT_i)^2$ in the basis $(\varphi_{\mathbf{k}}, \varphi_{-\mathbf{k}})$ has the form

$$\hat{U}_i\hat{U}_i^*=-\begin{bmatrix}\sigma_0 e^{2i\mathbf{k}\mathbf{a}_i} & 0\\ 0 & \sigma_0 e^{-2i\mathbf{k}\mathbf{a}_i}\end{bmatrix}. \tag{1}$$

(Here σ_0 is the 2×2 unit matrix.) The coefficient (-1) in front of the transformation matrix (1) is due to the fact that time reversal, applied twice to the spinor, changes its sign. Having solved Eq. 1, we find the matrices $\hat{U}_i$:

$$\hat{U}_i=\begin{bmatrix}0 & J\\ J^* & 0\end{bmatrix}, \quad J=i\sigma_y e^{i\mathbf{k}\mathbf{a}_i}, \tag{2}$$

or, in more convenient form:

$$\hat{U}_i=i\sigma_y(\cos(\mathbf{k}\mathbf{a}_i)\tau_x+\sin(\mathbf{k}\mathbf{a}_i)\tau_y). \tag{3}$$

Here τ_α, σ_α $(\alpha=1,2,3,0)$ are two sets of Pauli matrices. The matrices τ_α, σ_α act in the spaces $(\varphi_{\mathbf{k}}, \varphi_{-\mathbf{k}})$ and $(u_{\mathbf{k}}, v_{\mathbf{k}})$ respectively.

To understand how the new (magnetic) Brillouin zone is established, we note that the conditions

$$\hat{U}_i(\mathbf{k})=-\hat{U}_i\left(\mathbf{k}+\frac{\pi\mathbf{a}_i}{|\mathbf{a}_i|^2}\right), \tag{4}$$

$$\Lambda^{-1}\tau_0\hat{U}_i\tau_0\Lambda^*=-\hat{U}_i, \tag{5}$$

$$\Lambda=(\mathbf{n}\sigma), \tag{6}$$

are fulfilled, where $\mathbf{n}$ is a real unit vector. The relations 4–6 indicate that the spinor $\Lambda\psi_{\mathbf{k}}$ transforms according to the same representation as $\psi_{\mathbf{k}+\mathbf{Q}}$; here $\mathbf{Q}=\pi(\mathbf{a}_x+\mathbf{a}_y)/|\mathbf{a}|^2$. We note that the vector $\mathbf{Q}$ and the vectors differing from it by a period of the crystal reciprocal lattice $2\pi\mathbf{a}_i/|\mathbf{a}_i|^2$ are equivalent. Limiting the area of choice of $\mathbf{k}$ by the relationship $|k_x|+|k_y|<\pi/a$ (see the drawing), we find that the vectors $\mathbf{k}$ and $\mathbf{k}+\mathbf{Q}$ correspond to the same Brillouin zone. Thus, the set of spinors $\varphi_{\mathbf{k}}$ and $\Lambda\varphi_{\mathbf{k}+\mathbf{Q}}$ is a superposition of wave functions of two, generally different, energy bands. In order to find these accurate wave functions, it is also necessary to set up the spinors $\psi_{+,\mathbf{k}}$ and $\psi_{-,\mathbf{k}}$, which upon translation by a vector $\mathbf{Q}$: $\mathbf{k}\to\mathbf{k}+\mathbf{Q}$ transform to themselves, from $\varphi_{\mathbf{k}}$ and $\varphi_{\mathbf{k}+\mathbf{Q}}$. The most general form of such a basis is

$$\Psi_{\pm,\mathbf{k}}=\sin[\alpha(\mathbf{k})]\varphi_{\mathbf{k}}\pm\cos[\alpha(\mathbf{k})]\Lambda\varphi_{\mathbf{k}+\mathbf{Q}}, \tag{7}$$

with the additional conditions

$$\sin[\alpha(\mathbf{k}+\mathbf{Q})]=\cos[\alpha(\mathbf{k})], \quad \cos[\alpha(\mathbf{k}+\mathbf{Q})]=\sin[\alpha(\mathbf{k})].$$

Also,

$$\Psi_{\pm,\mathbf{k}+\mathbf{Q}}=\pm\Lambda\Psi_{\pm,\mathbf{k}}. \tag{8}$$

Relation 8 is the analog of the Bloch theorem.

The Hamiltonian corresponding to these two bands has the form

$$H^{(0)}=\sum_{(\mathbf{k})}[\varepsilon_+(\mathbf{k})\mathbf{a}_{+,\mathbf{k}}^+\mathbf{a}_{+,\mathbf{k}}+\varepsilon_-(\mathbf{k})\mathbf{a}_{-,\mathbf{k}}^+\mathbf{a}_{-,\mathbf{k}}]. \tag{9}$$

Here $\mathbf{a}_{\pm,\mathbf{k}}|0\rangle=\psi_{\pm,\mathbf{k}}$ and the summation is carried out over all vectors of the star in the Brillouin zone.

Physically, such a splitting of the spectrum into two branches, separated by an energy gap, occurs due to a doubling of the unit cell of the normal metal upon development of antiferromagnetic ordering. The Brillouin zone decreases by a factor of two (see the figure). We note that a similar reorganization of the spectrum does not occur for spinless particles described by single-value representations, as would be expected. Formally, this is expressed in the fact that for single-value representations the analog of relation 5 does not exist.

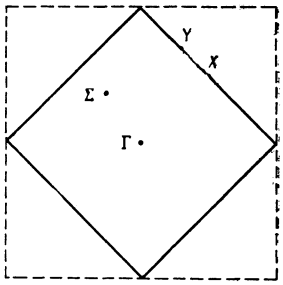

FIG. 1. Brillouin zone of an antiferromagnet (solid line) and of a normal metal (dashed line) with a square crystal lattice. Γ, Σ, *M*, *X*, and *Y* are characteristic points.

We now require that the matrix Λ have a similar form for all basis functions $\psi_{\mathbf{k}}$ belonging to different vectors **k** of the star {**k**}; that is, that it be invariant to the transformation of **k**-space under the action of D_4. We thereby identify a vector **n** with the direction of the antiferromagnetic order parameter, which is our approach is also invariant under D_4 and in general is a full invariant of the group $\mathcal{G}$.

We will examine an arbitrary point **k** in the Brillouin zone. The small group of this point is determined as the operations of the point group of symmetry s_m and D_4, under which the point **k** transforms either into itself, or into the equivalent at $2\pi\mathbf{a}_i/|\mathbf{a}_i|^2$, and also as the operations f_n of D_4, under which it transforms to a point displaced by **Q**. The operations $\{s_m\}$ and $\{f_n\}$ comprise the point group $P \subset D_4$; S is the group of operations $\{s_m\}$: $S \subset P$. According to Eq. (8) a representation of the operations f_n (in the general case a matrix $[f_n]$) is compounded with the matrix Λ acting in spin space; that is, it is a corepresentation. Therefore, a two-value irreducible representation of the small group of a given point is given by the matrices $\{[s_m], [f_n]\Lambda\}$; $[f_n]$, $[s_m]$ are the matrices of the irreducible representations of the group P, not involving the spin components of the system. These two-value irreducible representations can be decomposed in pairs in such a way that the matrices $[s_m]$ are identical for each pair, and the matrices corresponding to the elements f_n differ by a sign. As a consequence of Eq. (8), these representations correspond to two energy bands split by a gap formed when the antiferromagnetic ordering emerges. The set of matrices $[s_m]$ for each pair are representations of the group S, and are, generally speaking, reducible. Section 4 will deal with the description of representations for specific points on the Brillouin zone boundary. As an example, results are presented in the table for the point *M*.

3. A MAGNETIC FIELD

The two-value irreducible corepresentations of the group $\mathcal{G}$ at a generally situated point are two-dimensional. This fact, arising formally from the similarity of the representation matrices for operations RT, C_2 in the AFM and R, C_2 in the normal crystal with a square lattice (C_2 is the rotation by 180° about the fourfold axis), is the analog of the well-known Kramers-Eliot theorem, according to which twofold degeneracy exists in a crystal with inversion symmetry, due to its time-reversal symmetry. In a normal crystal the inclusion of a magnetic field removes this degeneracy, destroying RT-invariance. The destruction of RT-invariance in an antiferromagnet should also lead to splitting of the energy levels; however, the classification of states corresponding to these levels takes place not according to spin, but in terms of the two-value corepresentations.

Let the system be placed in an external magnetic field **h** or be perturbed by a ferromagnetic moment **M**. These cases are symmetrically indistinguishable; that is, they similarly lead to the destruction of RT-invariance: $RT\mathbf{h} = -\mathbf{h}$, $RT\mathbf{M} = -\mathbf{M}$. In the system Hamiltonian, together with Eq. (8) we introduce terms $\mathbf{a}_{\pm}^{+}, \mathbf{k}^{\sigma\alpha} \pm, \mathbf{k}$, which change sign upon RT-transformation, so that

$$H = H_0 + \sum_{\{\mathbf{k}\}} \mathbf{a}_{\pm,\mathbf{k}}^{+} (\mathbf{m}(\mathbf{k})\boldsymbol{\sigma})\, \mathbf{a}_{\pm,\mathbf{k}}. \tag{10}$$

Here $\mathbf{m}(\mathbf{k})$ is a vector in spin space which changes sign on RT-transformation. So, for example, in the approximation linear in **h**

$$m_i(\mathbf{k}) = g_{ij}(\mathbf{k}) H_j,$$

where $g_{ij}(\mathbf{k})$ is equivalent to the g-factor tensor.

According to the definition of the Brillouin zone, the Hamiltonian H should be invariant to $\mathbf{k} \to \mathbf{k} + \mathbf{Q}$, which occurs under the transform of Eq. (8). The condition of invariance of the Hamiltonian (10) means that the relation

$$(\boldsymbol{\sigma}\mathbf{n})\,(\mathbf{m}(\mathbf{k}+\mathbf{Q})\boldsymbol{\sigma})\,(\boldsymbol{\sigma}\mathbf{n}) = (\mathbf{m}(\mathbf{k})\boldsymbol{\sigma}), \tag{11}$$

must be fulfilled; that is,

$$[\mathbf{m}(\mathbf{k})\mathbf{n}]\,\boldsymbol{\sigma} + (\mathbf{m}(\mathbf{k})\mathbf{n}) = -[\mathbf{m}(\mathbf{k}+\mathbf{Q})\mathbf{n}]\,\boldsymbol{\sigma} + (\mathbf{m}(\mathbf{k}+\mathbf{Q})\mathbf{n}),$$

or, which is the same thing,

$$\mathbf{m}_{\parallel}(\mathbf{k}) = \mathbf{m}_{\parallel}(\mathbf{k}+\mathbf{Q}), \quad \mathbf{m}_{\perp}(\mathbf{k}) = -\mathbf{m}_{\perp}(\mathbf{k}+\mathbf{Q}), \tag{12}$$

where $\mathbf{m}_{\parallel}$ and $\mathbf{m}_{\perp}$ are components of **m** relative to **n**.

As seen from Eq. (12), the structure of the Hamiltonian (10) depends substantially on the position of **k** in the Brillouin zone. For any **k** the g-factors $g_{\parallel}(\mathbf{k})$ and $g_{\perp}(\mathbf{k})$ determining the Zeeman splitting in the fields $\mathbf{h}_{\parallel}$ and $\mathbf{h}_{\perp}$ are different. It is especially important that $g_{\perp}(\mathbf{k})$ goes to zero at all points where the vectors **k** and **k** + **Q** are identical; that is, at the boundary of the Brillouin zone[1)] (the solid line in the drawing). In this region, according to all the model theories, lie the most important electronic states. The vanishing of the perpendicular g-factors obviously principally affects the paramagnetic properties of the material, both statistical and EPR. The conclusions from the results formulated above in the weak-coupling model and a discussion of the experimental consequences are given in Ref. 12. From the point of view of applications the study of the selection rules for matrix elements of interband transitions $\psi_+ \to \psi_-$ is of significant interest. For operators invariant under RT-transformation (optical transitions, etc.) the selection rules do not differ from those for corresponding nonmagnetic lattices. In the case of operators changing their sign on RT-operations, the selection rules are contrary to the conditions (11) for intraband matrix elements, and just on the boundary of the magnetic zone transitions are allowed for vector values **d** perpendicular to **n** (or the corresponding tensor components) if they are odd under f_n operations. The result of this rule is analogous to the result of condition (11). We note that under the interchange $\mathbf{k} \Rightarrow \mathbf{k} + \mathbf{Q}$ the vector $\boldsymbol{\sigma}$ transforms as $\boldsymbol{\sigma} \Rightarrow 2(\boldsymbol{\sigma}\mathbf{n})\boldsymbol{\sigma} - \boldsymbol{\sigma}$. This relation is useful in writing the selec-

tion rules and the conditions of interaction with external fields.

We note that at several points of the Brillouin zone boundary the branches ψ_+ and ψ_- can mix. In this case the division of matrix elements into intra- and inter-band loses meaning, and both longitudinal and perpendicular components of the magnetic field give an interaction term. A detailed discussion of this problem for symmetry-induced degeneracy is given in Sec. 4.

In considering the case $\mathbf{h}_\parallel \neq 0$, we implicitly assume the presence of spin-orbital interactions. Without them we always have a configuration with $\mathbf{n}$ perpendicular to $\mathbf{h}$ (Ref. 13).

We do not consider orbital effects, assuming therefore that in the quasi-two-dimensional system the field lies in the conducting plane. In the general case the dispersion $g_\perp$ leads to interferences of the orbital and Zeeman quantization.[12] For instance, for a field perpendicular both to the plane and to $\mathbf{n}$, for states near the X point, the Zeeman term gives not a splitting of the Landau level, but a shift of the center of the orbit. This, obviously, results from the fact (see Ref. 12 or 13) that now a sign change in $\mathbf{h}$ is equivalent to a reflection of $\mathbf{k}$ about $\mathbf{Q}/2$.

4. SPECIAL POINTS OF THE BRILLOUIN ZONE BOUNDARY

We will examine in more detail a series of characteristic points of the Brillouin zone.

At a general point Y on the Brillouin zone boundary, the group S contains only the identity transform, and the P group includes also the rotation U_2' by 180° about the X-Y axis (see the drawing). The corepresentations of the small group $(\sigma_0, \pm\Lambda)$ correspond to two bands with wave functions $\psi_\pm$. A magnetic field $\mathbf{h}$ parallel to $\mathbf{n}$, according to Eq. 10, removes the twofold degeneracy of the spectrum, while a perpendicular field leaves the spectrum at the Y point twofold degenerate. Expansion of the Hamiltonian (9) in the vicinity of the Y point according to the $\mathbf{k}$-vector variation perpendicular $(\varkappa_\perp)$ and parallel $(\varkappa_\parallel)$ to the Brillouin zone boundary has the form

$$H=\varepsilon_\pm+(\alpha_\pm\varkappa_\perp^2+\beta_\pm\varkappa_\parallel)\mathbf{a}^+_{\pm,\varkappa}\mathbf{a}_{\pm,\varkappa}+\lambda_\pm(\mathbf{hn}) \times \mathbf{a}^+_{\pm,\varkappa}(\mathbf{n\sigma})\mathbf{a}_{\pm,\varkappa}+\gamma_\pm\varkappa_\perp[\mathbf{hn}]\mathbf{a}^+_{\pm,\varkappa}[\mathbf{n\sigma}]\mathbf{a}_{\pm,\varkappa}. \quad (13)$$

Here $\varepsilon_\pm$, $\alpha_\pm$, $\beta_\pm$, $\lambda_\pm$, and $\gamma_\pm$ are real coefficients.

At the X point the physical properties of the system are analogous to those examined earlier for the Y point. The difference lies only in the quadratic dependence of the energy on $\varkappa_\parallel$.

The point M, the corner of the magnetic Brillouin zone, has a richer symmetry. There, $S=D_2$ and $P=D_4$ hold (see the table). As is known, the group D_4 has four one-dimensional and one two-dimensional representations. The one-dimensional representations of D_4 are characterized by basis functions transforming as $(\xi, \eta = x \pm y)$

$$A_1 \propto 1, \quad B_1 \propto (\xi^2-\eta^2), \quad A_2 \propto \xi\eta(\xi^2-\eta^2), \quad B_2 \propto \xi\eta.$$

The corresponding two-dimensional corepresentations, as shown above, split into pairs (A_1B_1) and (A_2B_2). The corepresentations of each pair correspond to the upper and lower energy bands, separated by a gap.

Special consideration is necessary for the two-dimensional representation $E=\{\xi, \eta\}$ of the group D_4. Compounded with the matrices Λ, it guarantees fourfold degeneracy of the spectrum at the M-point, with basis functions

$$\psi_+=(\xi|\alpha\rangle, \eta|\beta\rangle), \quad \psi_-=(\eta|\alpha\rangle, \xi|\beta\rangle),$$

where $|\alpha\rangle$, $|\beta\rangle$ are the components of the two-value representation. Going away from the M point, the fourfold degeneracy is partially lifted, splitting into two double-valued one-dimensional representations ψ_+ and ψ_-.

Therefore, in the case of the E representation the AFM gap at the M point goes to zero. In analogy to the conclusions of Sec. 3, it can be shown that the interaction Hamiltonian with the magnetic field at the M point has the form

$$H=H_0+\mu(\mathbf{nh})\{\mathbf{a}_+^+(\mathbf{n\sigma})\mathbf{a}_+ + \mathbf{a}_-^+(\mathbf{n\sigma})\mathbf{a}_-\} + i\nu[\mathbf{nh}]\{\mathbf{a}_+^+[\mathbf{n\sigma}]\mathbf{a}_- - \mathbf{a}_-^+[\mathbf{n\sigma}]\mathbf{a}_+\}, \quad (14)$$

where μ, ν are real coefficients. We can persuade ourselves that for an arbitrary $\mathbf{h}$-direction the spectrum of the Hamiltonian (14) splits into two degenerate levels

$$\varepsilon=\varepsilon_0\pm[\mu^2\mathbf{h}_\parallel^2+\nu^2\mathbf{h}_\perp^2]^{1/2}.$$

5. SPIN-ORBIT INTERACTION

Up to now, only the exchange interaction between electron spins and magnetic moments on a lattice has been accounted for, as well as the exchange interaction between the moments themselves leading to antiferromagnetic ordering. This allowed examination of spin space rotations independently of coordinate space rotations, which, in part, was manifested in the arbitrary choice of direction of the vector $\mathbf{n}$

TABLE I. Two-dimensional A_1, A_2, B_1, B_2 and four-dimensional E corepresentations [$\mathscr{S}$] of the group $\mathscr{S}$ at the point M (analogs of the corresponding representations of the group $P=D_4$).

$\{D_2\}$	[$\mathscr{S}$]	E	C_2	$2U_2$	$2U_2'$	$2C_4$
A	A_1	1	1	1	$(\mathbf{n\sigma})$	$(\mathbf{n\sigma})$
	B_1	1	1	1	$-(\mathbf{n\sigma})$	$-(\mathbf{n\sigma})$
B_1	A_2	1	1	−1	$-(\mathbf{n\sigma})$	$(\mathbf{n\sigma})$
	B_2	1	1	−1	$(\mathbf{n\sigma})$	$-(\mathbf{n\sigma})$
B_2 B_3	E	$\begin{bmatrix}1&0\\0&1\end{bmatrix}$	$-\begin{bmatrix}1&0\\0&1\end{bmatrix}$	$\begin{bmatrix}1&0\\0&-1\end{bmatrix}$	$\begin{bmatrix}0&(\mathbf{n\sigma})\\(\mathbf{n\sigma})&0\end{bmatrix}$	$\begin{bmatrix}0&-(\mathbf{n\sigma})\\(\mathbf{n\sigma})&0\end{bmatrix}$

Note: In the first column representations of the group $S=D_2$ for the corresponding representations split by an energy gap are enumerated (see text for explanation).

in Eq. (6) in relation to coordinate space. Weak relativistic effects of spin-orbital interaction lead to linking of these two spaces and, generally speaking, destroy the invariance of the system Hamiltonian relative to the choice of **n**. This, in turn, can destroy the D_4 point group symmetry of the crystal. However, in an antiferromagnet with a square lattice these effects are small, since accounting for the relativistic corrections in first order does not change the classification of the electronic states. Such an interaction allows free rotation of spin space relative to coordinate space about the fourfold axis **C**. This is due to the absence of quadratic $(\mathbf{na}_x)^2$ and $(\mathbf{na}_y)^2$ terms in the expression for the anisotropic part of the free energy of the antiferromagnet, as well as the lack of connection of the electron spins with the $\mathbf{a}_x$ and $\mathbf{a}_y$ axes in first order in the spin-orbit interaction operator for the potential of a lattice with symmetry D_4.

The first order relativistic interaction fixes only the angle between the vector **n** and the **C** axis, which is equal to 90° or 0°. The magnetic moments either lie in the basal plane of the crystal, as happens in La_2CuO_4 (an easy-plane type antiferromagnet) or are aligned along the fourfold axis, as in La_2NiO_4. Taking account of higher approximations finally removes the unbroken degeneracy of the position of the **n** vector in coordinate space. Rotations of coordinate space cause rotations of spin space and the fourfold degenerate E representation is split up. So, for example, in the case of any easy axis E splits into two representations with basis functions

$$(x+iy)|\alpha\rangle,\ (x-iy)|\beta\rangle \text{ and } (x+iy)|\beta\rangle,\ (x-iy)|\alpha\rangle.$$

Other directions of **n** lower the D_4 point group symmetry of the crystal, and its magnetic group is one of the groups shown in Ref. 14.

[1)] This obviously does not agree with the corresponding result from the projection-operator method (see, for example, Ref. 11) for the strong-repulsion model.

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Translated by I. A. Howard