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Symmetry of the Wave Functions in the Band Theory of Ferromagnetic Metals*

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The symmetry of wave functions in the one-electron band theory of ferromagnetic solids is discussed. The exchange interaction, spin-orbit coupling, and coupling of spins to the magnetic induction vector **B** are included in the Hamiltonian. The resulting symmetry, which is not invariant under time reversal, can contain only those point operations which belong to the paramagnetic space group and leave the pseudo-vector **B** invariant at the same time. Character tables are presented for the case of face-centered cubic, body-centered cubic, and hexagonal close-packed structures and for various directions of **B**. Compatibility relations and lifting of degeneracies are discussed.

I. INTRODUCTION AND GENERAL THEORY

IN the last few years the band theory of solids has been considerably successful in explaining the properties of the ferromagnetic metals.[1] In particular the group-VIII transition metals Fe, Co, and Ni have been the subject of many investigations, both theoretical[2–12] as well as experimental,[13–19] which exhibit in a prominent way the band-theoretical aspects of the behavior of their conduction electrons.

It is important to remark, however, that in the ferromagnetic metals, which crystallize in the usual metallic structures fcc (Ni), bcc (Fe), and hcp (Co), the usual group-theoretical arguments,[20–22] which refer to non-magnetic materials, are no longer valid. For instance, the presence of a net magnetization results in the destruction of time-reversal symmetry[23] with the consequent splitting of up and down spin bands. The effects of the broken symmetries, moreover, go beyond this first-order and most important feature; in addition to time reversal, many other symmetry operations cease to exist in the presence of ferromagnetism. It is the purpose of this paper to reexamine the question of band symmetries in those circumstances and to provide the necessary character tables and compatibility relations which give complete information on the symmetry properties of the electronic states in ferromagnetic metals.

In the one-electron approximation, the electrons in a

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[1] For a complete reference to the many contributions to the itinerant electron theory of magnetism, see C. Herring, in *Magnetism*, edited by G. T. Rado and H. Suhl (Academic Press Inc., New York, 1966), Vol. 4.

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metal (magnetic or otherwise) are described by a set of one-particle wave functions that satisfy a self-consistent Schrödinger equation of the form

$$\mathcal{H}\psi_{n\mathbf{k}\sigma}=E_{n\sigma}(\mathbf{k})\psi_{n\mathbf{k}\sigma}, \quad (1)$$

where n denotes the band index, $\mathbf{k}$ the wave vector, and σ a generalized spin index. The Hamiltonian $\mathcal{H}$ can be decomposed into several contributions:

$$\mathcal{H}=\mathcal{H}_{\mathrm{K}}+\mathcal{H}_{\mathrm{Har}}+\mathcal{H}_{\mathrm{so}}+\mathcal{H}_{\mathrm{ex}}+\mathcal{H}_{B}, \quad (2)$$

where the various terms will be discussed in turn. The first two terms $\mathcal{H}_{\mathrm{K}}$ and $\mathcal{H}_{\mathrm{Har}}$ correspond to the kinetic energy and the Hartree self-consistent potential, respectively. $\mathcal{H}_{\mathrm{K}}$ has complete translational and rotational symmetry, while $\mathcal{H}_{\mathrm{Har}}$ is invariant under the operations of the space group of the relevant lattice structure (O_h^5 for face-centered cubic,[20] O_h^4 for body-centered cubic[20] and D_{6h}^4 for hexagonal close-packed[21]). The third term, $\mathcal{H}_{\mathrm{so}}$, is the usual spin-orbit interaction,[22] which is invariant under the space group operations applied simultaneously to spin and space coordinates. Therefore $(\mathcal{H}_{\mathrm{K}}+\mathcal{H}_{\mathrm{Har}}+\mathcal{H}_{\mathrm{so}})$ remains invariant under the operations of the pertinent "double" space group; it is also invariant under time-reversal symmetry.

The last two terms in (2), in the case of ferromagnetic metals, have a lower symmetry and consequently destroy many of the high-symmetry properties that are exhibited by the eigenfunctions of $(\mathcal{H}_{\mathrm{K}}+\mathcal{H}_{\mathrm{Har}}+\mathcal{H}_{\mathrm{so}})$. $\mathcal{H}_{\mathrm{ex}}$ is the usual Hartree-Fock exchange term which, when ferromagnetism is present, results in different energy levels for spin-up and spin-down electrons. It is important to emphasize that $\mathcal{H}_{\mathrm{ex}}$ distinguishes between up and down spins, which consequently have different energy spectra, but does not establish which direction in the crystal corresponds to the direction of quantization of spin. This preferred direction is determined mostly by the coupling between spin and magnetic induction $\mathbf{B}$ by the interaction

$$\mathcal{H}_{B}=-\mu_{B}\mathbf{B}\cdot\boldsymbol{\sigma}, \quad (3)$$

where μ_B is the Bohr magneton, $\boldsymbol{\sigma}$ the Pauli matrices, and $\mathbf{B}$ the magnetic induction vector. The spin-orbit term $\mathcal{H}_{\mathrm{so}}$ also contributes (although very weakly) to the determination of the direction of spin quantization.

If we make the usual approximation of taking $\mathbf{B}$ as constant throughout the crystal,[24] the term (3) has complete translational symmetry, but remains invariant only under those point operations (applied only to spin coordinates) that leave the pseudovector $\mathbf{B}$ invariant, i.e., the inversion, all rotations about the axis $\mathbf{B}$, and the product of these rotations and the inversion. The total Hamiltonian (2) therefore contains all the translations of the space group, but only those

[24] The approximation of constant $\mathbf{B}$ is not necessary for the group-theoretical arguments but makes the discussion simpler and easier to follow.

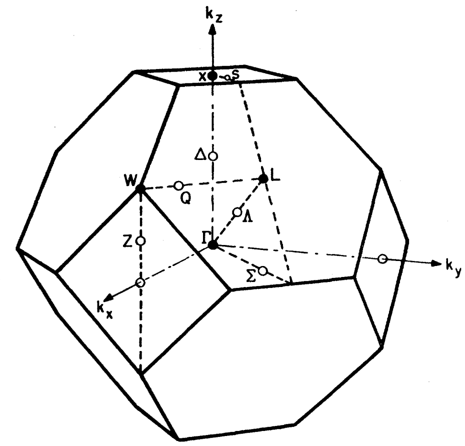

FIG. 1. First Brillouin zone for a fcc lattice. The major symmetry points and lines are designated according to the notation of Ref. 20.

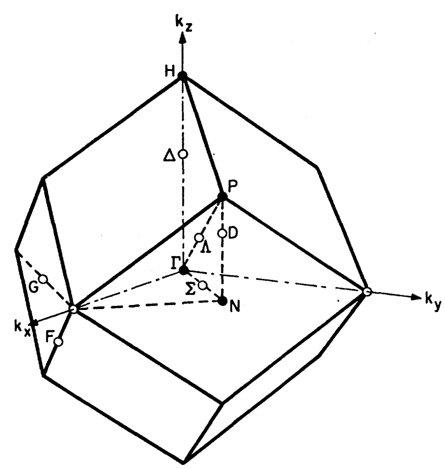

FIG. 2. First Brillouin zone for a bcc lattice. The major symmetry points and lines are designated according to the notation of Ref. 20.

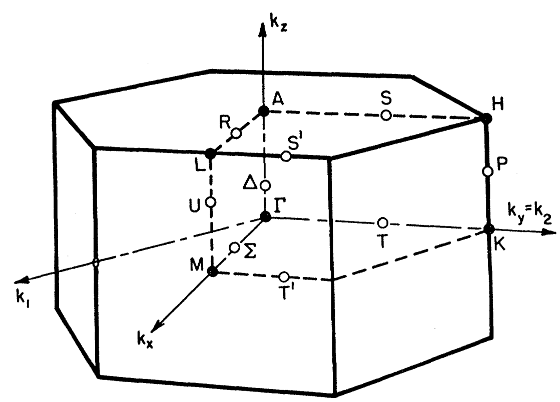

FIG. 3. First Brillouin zone for a hcp lattice. The major symmetry points and lines are designated according to the notation of Ref. 21.

rotations, rotation inversions, rotation translations, and rotation-inversion translations that belong to the double space group and leave the pseudovector **B** invariant. In addition, the presence of $(\mathcal{H}_{ex}+\mathcal{H}_B)$ removes time reversal as one of the symmetry operations of the Hamiltonian.

The discussion above shows clearly that of the 32 point groups only those that include rotations or rotation inversions about only one axis can be compatible with the symmetry of a ferromagnetic structure. This fact reduces the acceptable groups from 32 to 13, which are of the form C_n, C_{nh}, and S_n in the Schönflies notation or, equivalently, n, $\bar{n}$, and n/m in the international notation:

C_n:	C_1	C_2	C_3	C_4	C_6,
C_{nh}:	C_{1h}	C_{2h}	C_{3h}	C_{4h}	C_{6h},
S:		S_2		S_4	S_6.

All these groups (with the trivial exceptions of C_1 and C_{1h}) exhibit a preferential axis that corresponds to the direction of the magnetic induction **B**.

With this new classification of the total symmetry of the Hamiltonian, it is useful to analyze the usual simple approximations made in some ferromagnetic band structure calculations. The most common approximation[9,11,12,16,17] is to neglect the spin-orbit interaction $\mathcal{H}_{so}$. In that case there is no coupling between space and true spin coordinates. The space part of the Hamiltonian $(\mathcal{H}_K+\mathcal{H}_{Har}+\mathcal{H}_{ex})$ is invariant under *all* the operations of the single space group. The labels up and down spin simply identify two different bands that could be considered otherwise spinless. Time-reversal symmetry of course has been broken by $\mathcal{H}_{ex}$. The usual labeling by the single group representations[20,21] thus remains valid, and therefore many spurious degeneracies are still present.

When spin-orbit interaction is taken into account, it is necessary to consider $\mathcal{H}_B$ at the same time in order to have an unambiguous problem. The usual assumption in this case is to take the up-spin and down-spin bands as corresponding to directions parallel and antiparallel to **B**, respectively, the former labeling the majority spins and the latter the minority spins. $\mathcal{H}_B$ is neglected otherwise or its effects are included in $\mathcal{H}_{ex}$. It is a common approximation,[1,9] which describes some phenomena with good enough accuracy, to take $\mathcal{H}_{ex}$ as a constant for each spin. This produces a constant splitting ΔE between up-spin bands and down-spin bands, independent of the spatial part of the wave function. Such an approximation can be expressed by

$$(\mathcal{H}_{ex}+\mathcal{H}_B)_{app}=-\tfrac{1}{2}(\Delta E/|\mathbf{B}|)\mathbf{B}\cdot\boldsymbol{\sigma}, \quad (4)$$

which exhibits very clearly the invariance properties of the Hamiltonian which we have just discussed. Corrections to this model can easily be made by assuming that ΔE is a function of position **r**, a function of wave

TABLE I. Character table.

	E
γ_1	1

TABLE II. Character table.

	E	A
γ_1	1	i
γ_2	1	$-i$

TABLE III. Character table. $\omega=\frac{1}{2}(-1+i\sqrt{3})$.

	E	A	B
γ_1	1	-1	1
γ_2	1	$-\omega^2$	ω
γ_3	1	$-\omega$	ω^2

TABLE IV. Character table. $\alpha=(1+i)/\sqrt{2}$.

	E	A	B	C
γ_1	1	α	i	$-\alpha^*$
γ_2	1	α^*	$-i$	$-\alpha$
γ_3	1	$-\alpha$	i	α^*
γ_4	1	$-\alpha^*$	$-i$	α

TABLE V. Character table. $\omega=\frac{1}{2}(-1+i\sqrt{3})$.

	E	A	B	C	D	F
γ_1	1	i	-1	$-i$	1	i
γ_2	1	$-i$	-1	i	1	$-i$
γ_3	1	$-i\omega$	$-\omega^2$	i	ω	$-i\omega^2$
γ_4	1	$i\omega^2$	$-\omega$	$-i$	ω^2	$i\omega$
γ_5	1	$i\omega$	$-\omega^2$	$-i$	ω	$i\omega^2$
γ_6	1	$-i\omega^2$	$-\omega$	i	ω^2	$-i\omega$

TABLE VI. Character table.

	E	E_1	AA_1	BB_1	CC_1
γ_1	2	-2	0	0	0

TABLE VII. Character table. $\beta=1+i\sqrt{3}$.

	E	E_1	AA_1	B	B_1	CC_1	D	D_1	FF_1	JJ_1	KK_1	MM_1	PP_1	RR_1	LL_1
γ_1	2	-2	0	-2	2	0	2	-2	0	0	0	0	0	0	0
γ_2	2	-2	0	β	$-\beta$	0	$-\beta^*$	β^*	0	0	0	0	0	0	0
γ_3	2	-2	0	β^*	$-\beta^*$	0	$-\beta$	β	0	0	0	0	0	0	0

vector **k**, or, more generally, a nonlocal operator that depends on the angular momentum character of the wave function close to the ion sites. In all cases, however, ΔE exhibits the complete symmetry of the crystal lattice.

II. CHARACTER TABLES AND GENERAL RESULTS

In this section we give complete details of the group-theoretical properties of one-electron wave functions in ferromagnetic metals which crystallize in the fcc, bcc, and hcp structures and for various directions of magnetic induction **B**. For the cubic structures we follow the notation of Refs. 20 and 22. For the hexagonal structure the notation is identical to that of Refs. 21 and 22. Figure 1 shows the Brillouin zone for the fcc structure, Fig. 2 that of the bcc structure, and Fig. 3 that of the hcp lattice. Points and lines of symmetry are indicated and labeled. The results are given in tabular form and should be interpreted in the following way:

(a) Tables I–IX give the relevant double group character tables. The operations are expressed in a symbolic way that might take different meanings for different structures, magnetic induction directions, and symmetry points and that are properly defined in each case in Tables X–XVIII.

(b) Tables I–V correspond to those point groups G compatible with the ferromagnetic structure and such that they do not contain the inversion: C_1, C_2–C_{1h}, C_3, C_4–S_4, C_6–C_{3h}. To each of these tables we attach a companion character table (not actually displayed), labeled I_a–V_a, which corresponds to the direct product of the group G with the inversion group $S_2=\{E, J\}$. If the representations of G are labeled γ_i, $i=1, 2, \cdots, n$, then the representations of $G\otimes S_2$ are labeled $\gamma_i^{\pm}$, $i=1, 2, \cdots, n$, and such that

$$\gamma_i^{\pm}(R)=\gamma_i(R),$$
$$\gamma_i^{\pm}(JR)=\pm\gamma_i(R), \quad (5)$$

where R is any element in G. Tables I_a–V_a correspond to the groups S_2, C_{2h}, S_6, C_{4h}, and C_{6h}, respectively.

(c) Tables VI–IX appear in some representations of the nonsymmorphic group D_{6h}^4. They are not isomorphic to any point group.

(d) Tables X–XVIII give the proper character table, the definition of the operations, and the compatibility relations between the paramagnetic double group structure[22,25] and the ferromagnetic symmetries for the three crystal structures and magnetic inductions in various symmetry directions. The symmetry points, lines, and planes are identified in such a way as to distinguish between inequivalent ones in the presence of a magnetic induction **B**.

(e) For **B** in an arbitrary direction, no symmetry operations exist in general, except for translations. The proper representation for any point in the Brillouin zone is that of Table I. The only exceptions are points Γ, X, L, H, and N of the cubic structures and points Γ, A, M, and L of the hexagonal structure; these points have inversion symmetry and their representations correspond to Table I_a.

Some general and important features of these tables can be easily seen. Firstly, all ferromagnetic representations are one-dimensional, the only exceptions being the points A and L of the hcp structure for **B** parallel either to the [0001] axis or to $\langle 10\bar{1}0\rangle$ type directions. As a consequence, and with the exception of the points mentioned above, no degeneracy due to symmetry is permitted in the hcp structure, and none at all in the cubic cases.

Accidental degeneracies[26] are, however, allowed, but only when the magnetic induction **B** is parallel to a symmetry axis and in that case only along symmetry lines parallel to **B** or on symmetry planes perpendicular to **B**.

TABLE VIII. Character table.

	E	E_1	A	A_1
γ_1	1	-1	1	-1
γ_2	1	-1	-1	1

[25] The double representations of the Λ and F symmetry lines of the cubic structures are wrong in Ref. 22. The correct character tables are given in L. M. Falicov and S. Golin, Phys. Rev. **137**, A871 (1965), Table III.

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TABLE IX. Character table. $\omega=\frac{1}{2}(-1+i\sqrt{3})$.

	E	E_1	A	A_1	B	B_1	C	C_1	D	D_1	F	F_1
γ_1	1	-1	1	-1	-1	1	-1	1	1	-1	1	-1
γ_2	1	-1	-1	1	-1	1	1	-1	1	-1	-1	1
γ_3	1	-1	ω	$-\omega$	$-\omega^2$	ω^2	-1	1	ω	$-\omega$	ω^2	$-\omega^2$
γ_4	1	-1	ω^2	$-\omega^2$	$-\omega$	ω	-1	1	ω^2	$-\omega^2$	ω	$-\omega$
γ_5	1	-1	$-\omega$	ω	$-\omega^2$	ω^2	1	-1	ω	$-\omega$	$-\omega^2$	ω^2
γ_6	1	-1	$-\omega^2$	ω^2	$-\omega$	ω	1	-1	ω^2	$-\omega^2$	$-\omega$	ω

TABLE X. Character tables and compatibility relations for the fcc structure with the magnetic induction **B** parallel to the [001] direction.

Symmetry point	Character table	Corresponding elements	Representations
Γ	IV_a	$E=E,\ A=C_4,\ B=C_4^2,\ C=C_4^3$	$\Gamma_6^\pm\to\gamma_1^\pm+\gamma_2^\pm$ $\Gamma_7^\pm\to\gamma_3^\pm+\gamma_4^\pm$ $\Gamma_8^\pm\to\gamma_1^\pm+\gamma_2^\pm+\gamma_3^\pm+\gamma_4^\pm$
$X(1,0,0),\ X(0,1,0)$	II_a	$E=E,\ A=C_2$	$X_6^+,\ X_7^+\to\gamma_1^++\gamma_2^+$ $X_6^-,\ X_7^-\to\gamma_1^-+\gamma_2^-$
$X(0,0,1)$	IV_a	Same as Γ	$X_6^\pm\to\gamma_1^\pm+\gamma_2^\pm$ $X_7^\pm\to\gamma_3^\pm+\gamma_4^\pm$
$W(1,\frac{1}{2},0),\ W(-1,-\frac{1}{2},0)$ $W(\frac{1}{2},1,0),\ W(-\frac{1}{2},-1,0)$	II	$E=E,\ A=\sigma_h$	$W_6,\ W_7\to\gamma_1+\gamma_2$
$W(1,0,\frac{1}{2}),\ W(-1,0,-\frac{1}{2})$	IV	$E=E,\ A=JC_4,\ B=C_4^2,\ C=JC_4^3$	$W_6\to\gamma_1+\gamma_2$ $W_7\to\gamma_3+\gamma_4$
L	I_a	$E=E$	$L_4^+,\ L_5^+\to\gamma_1^+$ $L_4^-,\ L_5^-\to\gamma_1^-$ $L_6^\pm\to2\gamma_1^\pm$
$\Delta(0,0,a)$	IV	$E=E,\ A=C_4,\ B=C_4^2,\ C=C_4^3$	$\Delta_6\to\gamma_1+\gamma_2$ $\Delta_7\to\gamma_3+\gamma_4$
$\Sigma(a,a,0),\ \Sigma(-a,a,0)$	II	$E=E,\ A=\sigma_h$	$\Sigma_5\to\gamma_1+\gamma_2$
$S(a,a,1),\ S(a,-a,1)$	II	$E=E,\ A=\sigma_h$	$S_5\to\gamma_1+\gamma_2$
$Z(0,1,a),\ Z(1,0,a)$	II	$E=E,\ A=C_2$	$Z_5\to\gamma_1+\gamma_2$
$Z(1,a,0),\ Z(a,1,0)$ $Z(a,0,1),\ Z(0,a,1)$	II	$E=E,\ A=\sigma_h$	$Z_5\to\gamma_1+\gamma_2$
(001), Γ	II	$E=E,\ A=\sigma_h$	...
(001), X	II	$E=E,\ A=\sigma_h$	...

TABLE XI. Character tables and compatibility relations for the fcc structure with the magnetic induction **B** parallel to the [111] direction.

Symmetry point	Character table	Corresponding elements	Representations
Γ	III_a	$E=E,\ A=C_3,\ B=C_3^2$	$\Gamma_6^+,\ \Gamma_7^+\to\gamma_2^++\gamma_3^+$ $\Gamma_6^-,\ \Gamma_7^-\to\gamma_2^-+\gamma_3^-$ $\Gamma_8^\pm\to2\gamma_1^\pm+\gamma_2^\pm+\gamma_3^\pm$
X	I_a	$E=E$	$X_6^+,\ X_7^+\to2\gamma_1^+$ $X_6^-,\ X_7^-\to2\gamma_1^-$
$L(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	III_a	$E=E,\ A=C_3,\ B=C_3^2$	$L_4^\pm,\ L_5^\pm\to\gamma_1^\pm$ $L_6^\pm\to\gamma_2^\pm+\gamma_3^\pm$
$L(\frac{1}{2},\frac{1}{2},-\frac{1}{2}),\ L(\frac{1}{2},-\frac{1}{2},\frac{1}{2})$ $L(-\frac{1}{2},\frac{1}{2},\frac{1}{2})$	I_a	$E=E$	$L_4^\pm,\ L_5^\pm\to\gamma_1^\pm$ $L_6^\pm\to2\gamma_1^\pm$
$\Lambda(a,a,a)$	III	$E=E,\ A=C_3,\ B=C_3^2$	$\Lambda_4,\ \Lambda_5\to\gamma_1$ $\Lambda_6\to\gamma_2+\gamma_3$

TABLE XII. Character tables and compatibility relations for the fcc structure with the magnetic induction **B** parallel to the [110] direction.

Symmetry point	Character table	Corresponding elements	Representations
Γ	II_a	$E=E,\ A=C_2$	$\Gamma_6^\pm,\ \Gamma_7^\pm\to\gamma_1^\pm+\gamma_2^\pm$ $\Gamma_8^\pm\to 2\gamma_1^\pm+2\gamma_2^\pm$
$X(1,0,0)X(0,1,0)$	I_a	$E=E$	$X_6^\pm,\ X_7^\pm\to 2\gamma_1^\pm$
$X(0,0,1)$	II_a	$E=E,\ A=C_2$	$X_6^\pm,\ X_7^\pm\to\gamma_1^\pm+\gamma_2^\pm$
$W(1,0,\frac{1}{2}),\ W(-1,0,-\frac{1}{2})$	II	$E=E,\ A=C_2$	$W_6,\ W_7\to\gamma_1+\gamma_2$
$L(\frac{1}{2},\frac{1}{2},\frac{1}{2}),\ L(\frac{1}{2},\frac{1}{2},-\frac{1}{2})$	I_a	$E=E$	$L_4^\pm,\ L_5^\pm\to\gamma_1^\pm$ $L_6^\pm\to 2\gamma_1^\pm$
$L(\frac{1}{2},-\frac{1}{2},\frac{1}{2}),\ L(-\frac{1}{2},\frac{1}{2},\frac{1}{2})$	II_a	$E=E,\ A=C_2$	$L_4^\pm\to\gamma_1^\pm$ $L_5^\pm\to\gamma_2^\pm$ $L_6^\pm\to\gamma_1^\pm+\gamma_2^\pm$
$\Delta(0,0,a)$	II	$E=E,\ A=\sigma_h$	$\Delta_6\to\gamma_1+\gamma_2$ $\Delta_7\to\gamma_1+\gamma_2$
$\Lambda(a,-a,a),\ \Lambda(a,-a,-a)$	II	$E=E,\ A=\sigma_h$	$\Lambda_4\to\gamma_1$ $\Lambda_5\to\gamma_2$ $\Lambda_6\to\gamma_1+\gamma_2$
$\Sigma(a,a,0)$	II	$E=E,\ A=C_2$	$\Sigma_5\to\gamma_1+\gamma_2$
$\Sigma(-a,a,0)$	II	$E=E,\ A=\sigma_h$	$\Sigma_5\to\gamma_1+\gamma_2$
$S(a,a,1)$	II	$E=E,\ A=C_2$	$S_5\to\gamma_1+\gamma_2$
$S(a,-a,1)$	II	$E=E,\ A=\sigma_h$	$S_5\to\gamma_1+\gamma_2$
$Q(\frac{1}{2}+a,-\frac{1}{2}+a,\frac{1}{2})$ $Q(-\frac{1}{2}+a,\frac{1}{2}-a,-\frac{1}{2})$	II	$E=E,\ A=C_2$	$Q_3\to\gamma_1+\gamma_2$
$(110),\ \Gamma$	II	$E=E,\ A=\sigma_h$	...

TABLE XIII. Character tables and compatibility relations for the bcc structure with the magnetic induction **B** parallel to the [001] direction.

Symmetry point	Character table	Corresponding elements	Representations
Γ	IV_a	$E=E,\ A=C_4,\ B=C_4^2,\ C=C_4^3$	$\Gamma_6^\pm\to\gamma_1^\pm+\gamma_2^\pm$ $\Gamma_7^\pm\to\gamma_3^\pm+\gamma_4^\pm$ $\Gamma_8^\pm\to\gamma_1^\pm+\gamma_2^\pm+\gamma_3^\pm+\gamma_4^\pm$
H	IV_a	$E=E,\ A=C_4,\ B=C_4^2,\ C=C_4^3$	$H_6^\pm\to\gamma_1^\pm+\gamma_2^\pm$ $H_7^\pm\to\gamma_3^\pm+\gamma_4^\pm$ $H_8^\pm\to\gamma_1^\pm+\gamma_2^\pm+\gamma_3^\pm+\gamma_4^\pm$
$P(\frac{1}{2},\frac{1}{2},\frac{1}{2}),\ P(-\frac{1}{2},-\frac{1}{2},-\frac{1}{2})$	IV	$E=E,\ A=JC_4,\ B=C_4^2,\ C=JC_4^3$	$P_6\to\gamma_1+\gamma_2$ $P_7\to\gamma_3+\gamma_4$ $P_8\to\gamma_1+\gamma_2+\gamma_3+\gamma_4$
$N(\frac{1}{2},\frac{1}{2},0),\ N(-\frac{1}{2},\frac{1}{2},0)$	II_a	$E=E,\ A=C_2$	$N_5^\pm\to\gamma_1^\pm+\gamma_2^\pm$
$N(\frac{1}{2},0,\frac{1}{2}),\ N(\frac{1}{2},0,-\frac{1}{2})$ $N(0,\frac{1}{2},\frac{1}{2}),\ N(0,\frac{1}{2},-\frac{1}{2})$	I_a	$E=E$	$N_5^\pm\to 2\gamma_1^\pm$
$\Delta(0,0,a)$	IV	$E=E,\ A=C_4,\ B=C_4^2,\ C=C_4^3$	$\Delta_6\to\gamma_1+\gamma_2$ $\Delta_7\to\gamma_3+\gamma_4$
$\Delta(0,a,0),\ \Delta(a,0,0)$	II	$E=E,\ A=\sigma_h$	$\Delta_6,\ \Delta_7\to\gamma_1+\gamma_2$
$\Sigma(a,a,0),\ \Sigma(-a,a,0)$	I	$E=E$	$\Sigma_5\to 2\gamma_1$
$D(\frac{1}{2},\frac{1}{2},a)$	II	$E=E,\ A=C_2$	$D_5\to\gamma_1+\gamma_2$
$G(\frac{1}{2}-a,\frac{1}{2}+a,0)$ $G(-\frac{1}{2}+a,\frac{1}{2}+a,0)$	II	$E=E,\ A=\sigma_h$	$G_5\to\gamma_1+\gamma_2$
$(001),\ \Gamma$	II	$E=E,\ A=\sigma_h$	...

TABLE XIV. Character tables and compatibility relations for the bcc structure with the magnetic induction **B** parallel to the [111] direction.

Symmetry point	Character table	Corresponding elements	Representations
Γ	III_a	$E=E,\ A=C_3,\ B=C_3^2$	$\Gamma_6^\pm,\ \Gamma_7^\pm\to\gamma_2^\pm+\gamma_3^\pm$ $\Gamma_8^\pm\to2\gamma_1^\pm+\gamma_2^\pm+\gamma_3^\pm$
H	III_a	$E=E,\ A=C_3,\ B=C_3^2$	$H_6^\pm,\ H_7^\pm\to\gamma_2^\pm+\gamma_3^\pm$ $H_8^\pm\to2\gamma_1^\pm+\gamma_2^\pm+\gamma_3^\pm$
$P(\frac{1}{2},\frac{1}{2},\frac{1}{2}),\ P(-\frac{1}{2},-\frac{1}{2},-\frac{1}{2})$	III	$E=E,\ A=C_3,\ B=C_3^2$	$P_6,\ P_7\to\gamma_2+\gamma_3$ $P_8\to2\gamma_1+\gamma_2+\gamma_3$
N	I_a	$E=E$	$N_5^\pm\to2\gamma_1^\pm$
$\Lambda(a,a,a)$	III	$E=E,\ A=C_3,\ B=C_3^2$	$\Lambda_4,\ \Lambda_5\to\gamma_1$ $\Lambda_6\to\gamma_2+\gamma_3$
$F(-\frac{1}{2}+a,-\frac{1}{2}+a,\frac{1}{2}+a)$	III	$E=E,\ A=C_3,\ B=C_3^2$	$F_4,\ F_5\to\gamma_1$ $F_6\to\gamma_2+\gamma_3$

TABLE XV. Character tables and compatibility relations for the bcc structure with the magnetic induction **B** parallel to the [110] direction.

Symmetry point	Character table	Corresponding elements	Representations
Γ	II_a	$E=E,\ A=C_2$	$\Gamma_6^\pm,\ \Gamma_7^\pm\to\gamma_1^\pm+\gamma_2^\pm$ $\Gamma_8^\pm\to2\gamma_1^\pm+2\gamma_2^\pm$
H	II_a	$E=E,\ A=C_2$	$H_6^\pm,\ H_7^\pm\to\gamma_1^\pm+\gamma_2^\pm$ $H_8^\pm\to2\gamma_1^\pm+2\gamma_2^\pm$
$P(\frac{1}{2},\frac{1}{2},\frac{1}{2}),\ P(-\frac{1}{2},-\frac{1}{2},-\frac{1}{2})$	II	$E=E,\ A=\sigma_h$	$P_6,\ P_7\to\gamma_1+\gamma_2$ $P_8\to2\gamma_1+2\gamma_2$
$N(\frac{1}{2},\frac{1}{2},0),\ N(-\frac{1}{2},\frac{1}{2},0)$	II_a	$E=E,\ A=C_2$	$N_5^\pm\to\gamma_1^\pm+\gamma_2^\pm$
$N(\frac{1}{2},0,\frac{1}{2}),\ N(\frac{1}{2},0,-\frac{1}{2})$ $N(0,\frac{1}{2},\frac{1}{2}),\ N(0,\frac{1}{2},-\frac{1}{2})$	I_a	$E=E$	$N_5^\pm\to2\gamma_1^\pm$
$\Delta(0,0,a)$	II	$E=E,\ A=\sigma_h$	$\Delta_6,\ \Delta_7\to\gamma_1+\gamma_2$
$\Lambda(a,-a,a),\ \Lambda(a,-a,-a)$	II	$E=E,\ A=\sigma_h$	$\Lambda_4\to\gamma_1$ $\Lambda_5\to\gamma_2$ $\Lambda_6\to\gamma_1+\gamma_2$
$\Sigma(a,a,0)$	II	$E=E,\ A=C_2$	$\Sigma_5\to\gamma_1+\gamma_2$
$\Sigma(-a,a,0)$	II	$E=E,\ A=\sigma_h$	$\Sigma_5\to\gamma_1+\gamma_2$
$D(\frac{1}{2},\frac{1}{2},a),\ D(\frac{1}{2},-\frac{1}{2},a)$	II	$E=E,\ A=\sigma_h$	$D_5\to\gamma_1+\gamma_2$
$G(-\frac{1}{2}+a,\frac{1}{2}+a,0)$	II	$E=E,\ A=C_2$	$G_5\to\gamma_1+\gamma_2$
$G(\frac{1}{2}-a,\frac{1}{2}+a,0)$	II	$E=E,\ A=\sigma_h$	$G_5\to\gamma_1+\gamma_2$
$F(\frac{1}{2}-a,\frac{1}{2}-a,\frac{1}{2}+a)$ $F(-\frac{1}{2}+a,-\frac{1}{2}+a,\frac{1}{2}+a)$	II	$E=E,\ A=\sigma_h$	$F_4\to\gamma_1$ $F_5\to\gamma_2$ $F_6\to\gamma_1+\gamma_2$
(110), Γ	II	$E=E,\ A=\sigma_h$	···
(110), $N(\frac{1}{2},\frac{1}{2},0)$	II	$E=E,\ A=\sigma_h$	···

TABLE XVI. Character tables and compatibility relations for the hcp lattice with the magnetic induction **B** parallel to the [0001] direction.

Symmetry point	Character table	Corresponding elements	Representations
Γ	V_a	$E=\{\epsilon \mid 0\}$, $A=\{\delta_6 \mid \tau\}$, $B=\{\delta_3 \mid 0\}$ $C=\{\delta_2 \mid \tau\}$, $D=\{\delta_3^2 \mid 0\}$, $F=\{\delta_6^5 \mid \tau\}$	$\Gamma_7^\pm \rightarrow \gamma_3^\pm + \gamma_4^\pm$ $\Gamma_8^\pm \rightarrow \gamma_5^\pm + \gamma_6^\pm$ $\Gamma_9^\pm \rightarrow \gamma_1^\pm + \gamma_2^\pm$
A	VII	$E=\{\epsilon \mid 0\}$, $A=\{\delta_6 \mid \tau\}$, $B=\{\delta_3 \mid 0\}$ $C=\{\delta_2 \mid \tau\}$, $D=\{\delta_3^2 \mid 0\}$, $F=\{\delta_6^5 \mid \tau\}$ $J=\{i \mid \tau\}$, $K=\{\sigma_3 \mid 0\}$, $L=\{\sigma_3^5 \mid 0\}$ $M=\{\sigma_6 \mid \tau\}$, $P=\{\rho \mid 0\}$, $R=\{\sigma_6^5 \mid \tau\}$ $G_1=G\times\{\epsilon \mid t_1\}$ for all elements G.	$A_4 \rightarrow \gamma_1$ $A_5 \rightarrow \gamma_1$ $A_6 \rightarrow \gamma_2+\gamma_3$
M	II_a	$E=\{\epsilon \mid 0\}$, $A=\{\delta_2 \mid \tau\}$	$M_5^+ \rightarrow \gamma_1^+ + \gamma_2^-$ $M_5^- \rightarrow \gamma_1^- + \gamma_2^-$
L	VI	$E=\{\epsilon \mid 0\}$, $A=\{\delta_2 \mid \tau\}$, $B=\{i \mid \tau\}$ $C=\{\rho \mid 0\}$ $G_1=G\times\{\epsilon \mid t_1\}$ for all elements G.	$L_3 \rightarrow \gamma_1$ $L_4 \rightarrow \gamma_1$
K	V	$E=\{\epsilon \mid 0\}$, $B=\{\delta_3 \mid 0\}$, $D=\{\delta_3^2 \mid 0\}$ $C=\{\rho \mid 0\}$, $F=\{\sigma_3^{-5} \mid 0\}$, $A=\{\sigma_3^{-1} \mid 0\}$	$K_7 \rightarrow \gamma_1+\gamma_6$ $K_8 \rightarrow \gamma_2+\gamma_4$ $K_9 \rightarrow \gamma_3+\gamma_5$
H	V	Same as point K	H_4, $H_6 \rightarrow \gamma_3$ H_5, $H_7 \rightarrow \gamma_5$ $H_8 \rightarrow \gamma_1+\gamma_4$ $H_9 \rightarrow \gamma_2+\gamma_6$
$P(K)$, $P(H)$	III	$E=\{\epsilon \mid 0\}$, $A=\{\delta_3 \mid 0\}$, $B=\{\delta_3^2 \mid 0\}$	P_4, $P_5 \rightarrow \gamma_2$ $P_6 \rightarrow \gamma_1+\gamma_3$
$U(M)$	II	$E=\{\epsilon \mid 0\}$, $A=\{\delta_2 \mid \tau\}$	$U_5 \rightarrow \gamma_1+\gamma_2$
$U(L)$	VIII	$E=\{\epsilon \mid 0\}$, $A=\{\delta_2 \mid \tau\}$ $E_1=\{\epsilon \mid t_1\}$, $A_1=\{\delta_2 \mid \tau+t_1\}$	$U_5 \rightarrow \gamma_1+\gamma_2$
Σ	II	$E=\{\epsilon \mid 0\}$, $A=\{\rho \mid 0\}$	$\Sigma_5 \rightarrow \gamma_1+\gamma_2$
R	II	$E=\{\epsilon \mid 0\}$, $A=\{\rho \mid 0\}$	$R_5 \rightarrow \gamma_1+\gamma_2$
T	II	$E=\{\epsilon \mid 0\}$, $A=\{\rho \mid 0\}$	$T_5 \rightarrow \gamma_1+\gamma_2$
S	II	$E=\{\epsilon \mid 0\}$, $A=\{\rho \mid 0\}$	S_3, $S_4 \rightarrow \gamma_1$ S_2, $S_5 \rightarrow \gamma_2$
$\Delta(\Gamma)$	V	$E=\{\epsilon \mid 0\}$, $A=\{\delta_6 \mid \tau\}$, $B=\{\delta_3 \mid 0\}$ $C=\{\delta_2 \mid \tau\}$, $D=\{\delta_3^2 \mid 0\}$, $F=\{\delta_6^5 \mid \tau\}$	$\Delta_7(\Gamma) \rightarrow \gamma_3+\gamma_4$ $\Delta_8(\Gamma) \rightarrow \gamma_5+\gamma_6$ $\Delta_9(\Gamma) \rightarrow \gamma_1+\gamma_2$
$\Delta(A)$	IX	Same as $\Delta(\Gamma)$ $G_1=G\times\{\epsilon \mid t_1\}$ for all elements G.	$\Delta_7(A) \rightarrow \gamma_4+\gamma_5$ $\Delta_8(A) \rightarrow \gamma_3+\gamma_6$ $\Delta_9(A) \rightarrow \gamma_1+\gamma_2$
(0001), **Γ** (0001), A	II	$E=\{\epsilon \mid 0\}$, $A=\{\rho \mid 0\}$	...

TABLE XVII. Character tables and compatibility relations for the hcp lattice with the magnetic induction **B** parallel to the [10$\bar{1}$0] direction.

Symmetry point	Character table	Corresponding elements	Representations
Γ	II_a	$E=\{\epsilon\mid 0\}$, $A=\{\delta_2''\mid 0\}$	$\Gamma_7^+, \Gamma_8^+, \Gamma_9^+\rightarrow\gamma_1^++\gamma_2^+$ $\Gamma_7^-, \Gamma_8^-, \Gamma_9^-\rightarrow\gamma_1^-+\gamma_2^-$
A	VI	$E=\{\epsilon\mid 0\}$, $A=\{\delta_2''\mid 0\}$, $B=\{i\mid\tau\}$ $C=\{\rho''\mid\tau\}$, $E_1=\{\epsilon\mid t_1\}$, $A_1=\{\delta_2''\mid t_1\}$ $B_1=\{i\mid\tau+t_1\}$, $C_1=\{\rho''\mid\tau+t_1\}$	$A_4, A_5\rightarrow\gamma_1$ $A_6\rightarrow 2\gamma_1$
$M\,(\frac{1}{2}, 0, -\frac{1}{2}; 0)$	II_a	$E=\{\epsilon\mid 0\}$, $A=\{\delta_2''\mid 0\}$	$M_5^+\rightarrow\gamma_1^++\gamma_2^+$ $M_5^-\rightarrow\gamma_1^-+\gamma_2^-$
$M(0, \frac{1}{2}, -\frac{1}{2}; 0)$ $M(\frac{1}{2}, -\frac{1}{2}, 0; 0)$	I_a	$E=\{\epsilon\mid 0\}$	$M_5^+\rightarrow 2\gamma_1^+$ $M_5^-\rightarrow 2\gamma_1^-$
$L(\frac{1}{2}, 0, -\frac{1}{2}; \frac{1}{2})$	VI	Same as point A	$L_3, L_4\rightarrow\gamma_1$
$L(0, \frac{1}{2}, -\frac{1}{2}; \frac{1}{2})$ $L(\frac{1}{2}, -\frac{1}{2}, 0; \frac{1}{2})$	I_a	$E=\{\epsilon\mid 0\}$	$L_3, L_4\rightarrow\gamma_1^++\gamma_1^-$
K	II	$E=\{\epsilon\mid 0\}$, $A=\{\rho''\mid\tau\}$	$K_7, K_8, K_9\rightarrow\gamma_1+\gamma_2$
H	VIII	$E=\{\epsilon\mid 0\}$, $A=\{\rho''\mid\tau\}$ $E_1=\{\epsilon\mid t_1\}$, $A_1=\{\rho''\mid\tau+t_1\}$	$H_4, H_7\rightarrow\gamma_1$ $H_5, H_6\rightarrow\gamma_2$ $H_8, H_9\rightarrow\gamma_1+\gamma_2$
$\Delta(\Gamma)$	II	$E=\{\epsilon\mid 0\}$, $A=\{\rho_2''\mid\tau\}$	$\Delta_7, \Delta_8, \Delta_9\rightarrow\gamma_1+\gamma_2$
$\Delta(A)$	VIII	Same as for point H	$\Delta_7, \Delta_8, \Delta_9\rightarrow\gamma_1+\gamma_2$
$\Sigma(a, 0, -a; 0)$	II	$E=\{\epsilon\mid 0\}$, $A=\{\delta_2''\mid 0\}$	$\Sigma_5\rightarrow\gamma_1+\gamma_2$
$T(a, -2a, a; 0)$ $T'(\frac{1}{2}+a, -2a, -\frac{1}{2}+a; 0)$	II	$E=\{\epsilon\mid 0\}$, $A=\{\rho_2''\mid\tau\}$	$T_5\rightarrow\gamma_1+\gamma_2$
$R(a, 0, -a; \frac{1}{2})$	II	$E=\{\epsilon\mid 0\}$, $A=\{\delta_2''\mid 0\}$	$R_5\rightarrow\gamma_1+\gamma_2$
$S(a, -2a, a; \frac{1}{2})$ $S'(\frac{1}{2}+a, -2a, -\frac{1}{2}+a; \frac{1}{2})$	VIII	Same as for point H	$S_2, S_4\rightarrow\gamma_1$ $S_3, S_5\rightarrow\gamma_2$
$P(K)$	II	$E=\{\epsilon\mid 0\}$, $A=\{\rho''\mid\tau\}$	$P_4(K)\rightarrow\gamma_2$ $P_5(K)\rightarrow\gamma_1$ $P_6(K)\rightarrow\gamma_1+\gamma_2$
$P(H)$	VIII	Same as for point H	$P_4(H)\rightarrow\gamma_1$ $P_5(H)\rightarrow\gamma_2$ $P_6(H)\rightarrow\gamma_1+\gamma_2$
$U(M)\,(\frac{1}{2}, 0, -\frac{1}{2}; a)$	II	$E=\{\epsilon\mid 0\}$, $A=\{\rho_2''\mid\tau\}$	$U_5(M)\rightarrow\gamma_1+\gamma_2$
$U(L)\,(\frac{1}{2}, 0, -\frac{1}{2}; a)$	VIII	Same as for point H	$U_5(L)\rightarrow\gamma_1+\gamma_2$
$(10\bar{1}0)$, Γ $(10\bar{1}0)$, $M(\frac{1}{2}, 0, -\frac{1}{2}; 0)$	II or VIII	Same as for line U or Δ	···

TABLE XVIII. Character tables and compatibility relations for the hcp lattice with the magnetic induction **B** parallel to the [11$\bar{2}$0] direction.

Symmetry point	Character table	Corresponding elements	Representations
Γ	II_a	$E=\{\epsilon\,\vert\,0\}$, $A=\{\delta_2'\,\vert\,\tau\}$	$\Gamma_7^+, \Gamma_8^+, \Gamma_9^+ \to \gamma_1^+ + \gamma_2^+$ $\Gamma_7^-, \Gamma_8^-, \Gamma_9^- \to \gamma_1^- + \gamma_2^-$
A	II_a	Same as Γ	$A_4 \to \gamma_1^+ + \gamma_1^-$ $A_5 \to \gamma_2^+ + \gamma_2^-$ $A_6 \to \gamma_1^+ + \gamma_1^- + \gamma_2^+ + \gamma_2^-$
$M(\frac{1}{2}, -\frac{1}{2}, 0; 0)$	II_a	Same as Γ	$M_5^+ \to \gamma_1^+ + \gamma_2^+$ $M_5^- \to \gamma_1^- + \gamma_2^-$
$M(\frac{1}{2}, 0, -\frac{1}{2}; 0)$ $M(0, \frac{1}{2}, -\frac{1}{2}; 0)$	I_a	$E=\{\epsilon\,\vert\,0\}$	$M_5^+ \to 2\gamma_1^+$ $M_5^- \to 2\gamma_1^-$
$L(\frac{1}{2}, -\frac{1}{2}, 0; \frac{1}{2})$	II_a	Same as Γ	$L_3 \to \gamma_1^+ + \gamma_1^-$ $L_4 \to \gamma_2^+ + \gamma_2^-$
$L(\frac{1}{2}, 0, -\frac{1}{2}; \frac{1}{2})$ $L(0, \frac{1}{2}, -\frac{1}{2}; \frac{1}{2})$	I_a	$E=\{\epsilon\,\vert\,0\}$	$L_3, L_4 \to \gamma_1^+ + \gamma_1^-$
K	II	$E=\{\epsilon\,\vert\,0\}$, $A=\{\delta_2'\,\vert\,\tau\}$	$K_7, K_8, K_9 \to \gamma_1 + \gamma_2$
H	II	Same as K	$H_4, H_5 \to \gamma_1$ $H_6, H_7 \to \gamma_2$ $H_8, H_9 \to \gamma_1 + \gamma_2$
$\Delta(0, 0, 0; a)$	II	$E=\{\epsilon\,\vert\,0\}$, $A=\{\rho_2'\,\vert\,0\}$	$\Delta_7, \Delta_8, \Delta_9 \to \gamma_1 + \gamma_2$
$U(\frac{1}{2}, -\frac{1}{2}, 0; a)$	II	$E=\{\epsilon\,\vert\,0\}$, $A=\{\rho_2'\,\vert\,0\}$	$U_5 \to \gamma_1 + \gamma_2$
$\Sigma(a, -a, 0; 0)$	II	$E=\{\epsilon\,\vert\,0\}$, $A=\{\rho_2'\,\vert\,0\}$	$\Sigma_5 \to \gamma_1 + \gamma_2$
$R(a, -a, 0; \frac{1}{2})$	II	$E=\{\epsilon\,\vert\,0\}$, $A=\{\rho_2'\,\vert\,0\}$	$R_5 \to \gamma_1 + \gamma_2$
$T(a, a, -2a; 0)$ $T'(\frac{1}{2}+a, -\frac{1}{2}+a, -2a; 0)$	II	$E=\{\epsilon\,\vert\,0\}$, $A=\{\delta_2'\,\vert\,\tau\}$	$T_5 \to \gamma_1 + \gamma_2$
$S(a, a, -2a; \frac{1}{2})$ $S'(\frac{1}{2}+a, -\frac{1}{2}+a, -2a; \frac{1}{2})$	II	$E=\{\epsilon\,\vert\,0\}$, $A=\{\delta_2'\,\vert\,\tau\}$	$S_2, S_3 \to \gamma_1$ $S_4, S_5 \to \gamma_2$
$(11\bar{2}0)$, Γ	II	$E=\{\epsilon\,\vert\,0\}$, $A=\{\rho_2'\,\vert\,0\}$	...

It is interesting to remark that the sticking together of the bands at the AHL plane of the hcp Brillouin zone is completely removed, with the possible exception of the points A and L. The line R, which in the paramagnetic structure is fourfold degenerate (including spin) because of time-reversal symmetry, does not split into two double levels (as it would be predicted by the breaking of time-reversal symmetry only), but rather into four single levels. Similar considerations apply to all other symmetry points and lines in the three structures here discussed.

It is also worth pointing out that the ferromagnetic band structures, in general, should be consistent with the fact that very few accidental degeneracies are permitted. Consequently, the presence of spin-orbit coupling removes most of the band crossovers, and in particular, intersections of up-spin and down-spin bands should result in degeneracies being lifted with a consequent hybridization of the separate spin systems. Effects of this kind have been found in ferromagnetic Ni [17,19] and will be discussed in a subsequent paper.[27]

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[27] J. Ruvalds and L. M. Falicov, following paper, Phys. Rev. **172**, 508 (1968).