Superconducting band stabilizing superconductivity in MgB$_2$

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It is shown that the superconducting intermetallic compound MgB$_2$ possesses a narrow, partly filled “superconducting band” with Wannier functions of special symmetry in its band structure. This result corroborates previous observations about the band structures of numerous superconductors and non-superconductors showing that evidently superconductivity is always connected with such superconducting bands. These findings are interpreted in the framework of a nonadiabatic extension of the Heisenberg model. Within this new group-theoretical model of correlated systems, Cooper pairs are stabilized by a nonadiabatic mechanism of constraining forces effective in narrow superconducting bands. The formation of Cooper pairs in a superconducting band is mediated by the energetically lowest boson excitations in the considered material that carry the crystal spin-angular momentum $1 \cdot \hbar$. These crystal-spin-1 bosons are proposed to determine whether the material is a conventional low-$T_c$ or a high-$T_c$ superconductor. This interpretation provides the electron-phonon mechanism that enters the BCS theory in conventional superconductors.

Keywords: occurrence of superconductivity, superconducting band, correlated electrons, nonadiabatic Heisenberg model, group theory

1. INTRODUCTION

In a former paper [1] the author proposed to generalize the classical Heisenberg model of magnetism [2] by introducing three new postulates emphasizing the atomic-like motion of electrons in narrow, partly filled energy bands. The resulting “nonadiabatic Heisenberg model” (NHM) uses the term “atomic-like motion” in the sense of Mott [3] and Hubbard [4]: as long as possible the electrons occupy localized states and perform their band motion by hopping from one atom to another.

This group-theoretical model provides a novel concept to understand correlation effects in narrow bands in terms of symmetry-adapted Wannier functions and was developed to interpret the existence of magnetic and superconducting bands with Wannier functions of special symmetries in the band structures of magnetic and superconducting materials.

Evidently, the magnetic states in Cr [5], Fe [6], La$_2$CuO$_4$ [7], and YBa$_2$Cu$_3$O$_6$ [8] are connected with narrow, partly filled magnetic bands in the band structures of the respective materials. Superconducting bands (as shall be defined in Sec. 3.1) have already been identified in the band structures of numerous elemental superconductors [9] and of the high-temperature superconductors La$_2$CuO$_4$ [7] and YBa$_2$Cu$_3$O$_7$ [10]. Furthermore, partly filled superconducting bands cannot be found in those elemental metals (such as Li, Na, K, Rb, Cs, Ca, Cu, Ag, and Au) which do not become superconducting [2]. An investigation into the band structures of the transition metals in terms of superconducting bands straightforwardly leads to the Matthias rule [11].

The aim of the present paper is to show that the intermetallic compound MgB$_2$ with the relatively high transition temperature $T_c \approx 39 K$ [12] possesses a narrow, partly filled superconducting band in its band structure. Before in Sec. 3 the existence of this band shall be established, the following Sec. 2 outlines the physical substance of the new nonadiabatic model and Sec. 3 gives the definition of superconducting bands and a short characterization of the mechanism of Cooper pair formation in these bands.

2. NONADIABATIC HEISENBERG MODEL

In this section the nonadiabatic Heisenberg model is shortly characterized, a detailed substantiation of all the statements is given in Ref. [1].

Within the NHM, the Hamiltonian

$$H^n = H_{HF} + H^n_{Cb}$$

in a partly filled superconducting or magnetic band consists of the familiar Hartree-Fock operator $H_{HF}$ and the nonadiabatic Coulomb interaction

$$H^n_{Cb} = \sum_{T,m} \langle T_1, m_1; n; T_2, m_2, n | H_{Cb} | T_1', m_1', n; T_2', m_2', n \rangle$$

$$\times c_{T_1, m_1}^{n \dagger} c_{T_2, m_2}^{n \dagger} c_{T_1', m_1'}^{n} c_{T_2', m_2'}^{n}.$$  (2.2)

The fermion operators $c_{T,m}^{n \dagger}$ and $c_{T,m}^{n}$ create and annihilate electrons in “nonadiabatic localized states” $| T, m, n \rangle$ [with crystal spin $m$ (see Sec. 2.1.3)] on the atom at position $T$ that depend on an additional quantum number $n$ labeling different states of the nonadiabatic motion of the center of mass of the localized states [13]. The matrix elements of $H^n_{Cb}$ are integrals over nonadiabatic localized functions as given in Eq. (2.17) of Ref. [1].

The introduction of these nonadiabatic localized states allows a realistic description of an atomic-like motion of the electrons. While in the framework of the adiabatic approximation the electrons move in rigid orbitals in the average potential of the other electrons, in the nonadiabatic system a localized electron moves in a potential depending on which of the adjacent localized states is occupied and on the present motion of the electrons in
these states. Such a correlated electronic motion within a fluctuating potential leads to localized orbitals which are not symmetric at any moment, but only on the average of time. As a consequence, the centers of mass of the localized states become permanently accelerated in varying directions. The resulting nonadiabatic motions of the centers of mass are labeled by the new quantum number \( n \).

The NHM assumes that there exist nonadiabatic localized states satisfying the equation

\[
\langle T_1, m_1, n; T_2, m_2, n | H_{C6} | T_1', m_1', n; T_2', m_2', n \rangle = 0
\]

(2.3)

for

\[
\{ T_1, T_2 \} \neq \{ T_1', T_2' \}
\]

(2.4)

if the considered partly filled band is one of the narrowest bands of the given material, where \( \{ T_1, T_2 \} = \{ T_1', T_2' \} \) means \( T_1 = T_1' \) and \( T_2 = T_2' \) or \( T_1 = T_2' \) and \( T_2 = T_1' \).

This Eq. (2.3) follows from the first postulate of the NHM which assumes that the correlation effects specified by Eq. (2.4) are energetically unfavorable in narrow, partly filled bands. So the electrons modify their localized orbitals within the nonadiabatic localized states in such a way that the transitions specified by Eq. (2.4) do not occur. These modified electronic orbitals yield a well-defined motion of the centers of mass labeled by the quantum number \( n \).

Eq. (2.3) defines the “atomic-like state of motion” within the NHM and replaces the stronger Heisenberg energy by the “nonadiabatic condensation energy”

\[
\Delta E = E_b - E_a
\]

(2.5)

at the transition from the adiabatic (more bandlike) to the nonadiabatic atomic-like state. \( E_a \) and \( E_b \) denote the ground-state energies of the operator \( H^n \) in Eq. (2.1) and of the related operator within the adiabatic approximation, respectively. \( \Delta E \) may be approximated by Eq. (2.20) of Ref. [1].

2.1. Novel features of the nonadiabatic Heisenberg model

A correlated electron system characterized by Eq. (2.3) possesses three novel features distinguishing it from any system described within the adiabatic approximation. First, within the NHM there exists a “nonadiabatic condensation energy” \( \Delta E \); second, the nonadiabatic Hamiltonian \( H^n \) possesses unusual commutation properties; and thirdly, the “crystal spin” of the nonadiabatic localized states is a conserved quantity.

2.1.1. Nonadiabatic condensation energy

Eq. (2.3) is assumed to be satisfied in the ground state of the narrowest, partly filled bands of the metals. Since this equation is clearly not true within the adiabatic approximation, the Coulomb correlation energy of the nonadiabatic atomic-like state characterized by Eq. (2.3) is lower than the correlation energy of this state within the adiabatic approximation. Hence, the electrons of the narrowest, partly filled bands of the metals lower their energy by the “nonadiabatic condensation energy”

\[
\Delta E = E_b - E_a
\]

(2.5)

In superconducting and magnetic bands the symmetry of the nonadiabatic localized states is not adapted to the space group \( G \) of the considered material, but only to a subgroup \( M \) of \( G \). As a consequence of Eq. (2.3), the nonadiabatic Hamiltonian \( H^n \) in Eq. (2.1) commutes with all the symmetry operators of \( M \), but not with the symmetry operators of \( G \) that do not belong to \( M \). Thus, the group-theoretical NHM allows a straightforward physical interpretation of the symmetry of the localized states related to the atomic-like motion in narrow, partly filled bands.

This feature distinguishes \( H^n \) from any Hamiltonian \( H \) written in the adiabatic approximation since the symmetry properties of \( H \) are independent of the symmetry of the Wannier basis used to calculate its matrix elements.

2.1.2. Commutation properties of the nonadiabatic Hamiltonian \( H^n \)

The nonadiabatic localized states are no longer labeled by the spin quantum number \( s = \frac{1}{2} \), but by a new quantum number \( m = \pm \frac{1}{2} \) which may be called the quantum number of the “crystal spin”. This is in analogy to the wave vector \( \mathbf{k} \) of the Bloch functions which is sometimes referred to as “crystal momentum” in order to distinguish it from a true momentum.

Within the nonadiabatic correlated system the conservation law of spin angular momentum as expressed by the equation

\[
[H, S(\alpha)] = 0 \quad \text{for } \alpha \in O(3)
\]

(2.6)

is replaced by the conservation law

\[
[H^n, M(\alpha)] = 0 \quad \text{for } \alpha \in G_M
\]

(2.7)

of the crystal spin \( m \). The operators \( S(\alpha) \) are the symmetry operators of the electron spin and \( O(3) \) stands for the three-dimensional rotation group; \( M(\alpha) \) and \( G_M \) denote the analogous operators and the corresponding group, respectively, in the space group of the considered material.

At interactions of the electrons with phonons, a Bloch state bears the crystal-spin angular momentum \( m = \frac{1}{2} \cdot \hbar \) and suitable linear combinations of the phonons carry the crystal spin \( m = 1 \cdot \hbar \).
2.2. Superconducting and magnetic bands

Localized functions \((r, t, q | T, m, n)\) representing the nonadiabatic localized states are highly complicated since they depend on an additional coordinate \(q\) related to the nonadiabatic motion of the center of mass (while \(r\) and \(t\) denote, as usual, the local and spin coordinate, respectively, of the localized electron). Fortunately, these functions need not to be known. The NHM only postulates their existence and assumes that they have the same symmetry and spin dependence as the best localized exact Wannier functions of the considered partly filled energy band. In this context, “exact Wannier functions” form a complete basis of the Bloch functions of this band.

In several narrow, partly filled energy bands of the metals the electrons can gain the nonadiabatic condensation energy \(\Delta E\) only under specific conditions: in a narrow, partly filled “magnetic band” \([1, 8]\) related to a magnetic structure \(S\) the electrons can occupy the atomic-like state only if this magnetic structure \(S\) actually exists in the considered material. Further, electrons in a narrow, partly filled “superconducting band” (as defined in Sec. 3.1) occupying the atomic-like state are forced in a new way to form Cooper pairs below a certain transition temperature. This “new way” will be substantiated in Sec. 3.2.

This result suggests that the nonadiabatic condensation energy \(\Delta E\) in Eq. (2.5) stabilizes both magnetism \([2, 4]\) and superconductivity \([14, 15]\). Both phenomena have the same physical origin: they exist because the electrons at the Fermi level tend to occupy the energetically favorable atomic-like state. The special symmetry and spin dependence of the related Wannier function determine whether the material becomes magnetic or superconducting (or has a property not yet considered). This important statement of the NHM is corroborated by the calculated band structures mentioned in Sec. 2.2.

3. SUPERCONDUCTING BANDS AND SUPERCONDUCTIVITY

3.1. Definition of superconducting bands

Usually, the energy bands crossing the Fermi level in the paramagnetic metals are degenerate at several points and lines of symmetry of the Brillouin zone. Therefore, it is not possible to separate narrow isolated sets of bands whose Bloch functions can be unitarily transformed into best localized Wannier functions that are symmetry-adapted to the full space group \(G\) of the considered metal. However, in some cases such Wannier functions may be constructed if we allow that they are adapted only to the symmetry of a magnetic subgroup \(M\) of \(G\) or if they are allowed to be spin dependent \([1]\). In the first case, the band is a magnetic band as mentioned in the foregoing Sec. 2.2 in the second case it is a superconducting band.

We define an energy band of a given material to be a “superconducting band” if the Bloch functions of this band can be unitarily transformed into spin-dependent Wannier functions \(w_{im}(r - R - \rho_i, t)\) (as defined by Eq. (A22) of Ref. [1]) which are

- centered on a (well-defined) part of the atoms (at positions \(T = R + \rho_i\));
- symmetry-adapted to the (full) space group \(G\) of this material;
- labeled by the quantum number \(m = \pm \frac{1}{2}\) of the crystal spin [see note (ii) of Table IV]; and
- localized as well as possible.

3.2. Mechanism of Cooper pair formation in a superconducting band

In a narrow, roughly half-filled superconducting band, the electron system has no other possibility to gain the nonadiabatic condensation energy \(\Delta E\) in Eq. (2.5) but to occupy an atomic-like state represented by spin-dependent Wannier functions. This spin dependence has far reaching consequences because only special atomic-like motions with spin-dependent localized states may exist in the nonadiabatic system. These states are determined by the interplay of two conservation laws: on the one hand, the bare electrons satisfy the conservation of the electron spin and, on the other hand, the nonadiabatic localized states conserve the crystal spin.

In this section, the atomic-like motion with spin-dependent localized states is shortly characterized, a detailed substantiation of all the statements is given in Ref. [15].

3.2.1. Nonadiabatic atomic-like motion with spin-dependent localized states

When the localized states are represented by spin-dependent Wannier functions, the nonadiabatic operator \(H_{cb}^0\) of Coulomb interaction complying with Eq. (2.3) does not conserve the crystal spin angular momentum, i.e.,

\[ [H_{cb}^0, M(\alpha)] \neq 0 \]  

for at least one \(\alpha \in G_M\). At first sight, this result seems to show that the NHM is not applicable to superconducting bands. However, the nonadiabatic motion of the centers of mass in the localized states gives point to another interpretation. Remember that the quantum number \(n\) in Eq. (2.3) labels the special nonadiabatic motion of the centers of mass of those localized states which satisfy this Eq. (2.3). Thus, Eq. (3.1) indicates that this special nonadiabatic motion occurs in such a way that phonons or other boson excitation are excited (or absorbed) which...
Coulomb interaction $H$ with $H$ nonadiabatic Hamiltonian determined by Eq. (4.28) of Ref. [14]. The complete band. In cubic crystals the matrix elements of $H^{ns}$ with crystal spin $b$

store the surplus crystal spin angular momenta. This interpretation is corroborated by the fact that by the mere addition of symmetrized boson operators we may construct from $H^{ns}_{Cb}$ an interaction

$$
H^{ns}_{Cb} = \sum_{T,m} \langle T', l_1; T_2, l_2; T_1, m_1, n; T_2, m_2, n | H_{Cb} | T_1, m_1', n; T_2, m_2', n \rangle b_{T_1 l_1}^\dagger b_{T_2 l_2}^\dagger \times c_{T_1 m_1}^\dagger c_{T_2 m_2}^\dagger c_{T_1 m_1'} c_{T_2 m_2'} + H.c. \tag{3.2}
$$

which conserves the crystal spin,

$$[H^{ns}_{Cb}, M(\alpha)] = 0 \quad \text{for } \alpha \in G_M. \tag{3.3}$$

The boson operator $b_{Tl}^\dagger$ creates a localized boson $|T, l\rangle$ with crystal spin $l = -1, 0, +1$ at the position $T$.

This “spin-boson interaction” $H^{ns}_{Cb}$ replaces the Coulomb interaction $H^0_{Cb}$ in a narrow superconducting band. In cubic crystals the matrix elements of $H^{ns}_{Cb}$ are determined by Eq. (4.28) of Ref. [14]. The complete nonadiabatic Hamiltonian $H^n$ now may be written as

$$H^n = H_{HF} + H^{ns}_{Cb} + H_b \tag{3.4}$$

with $H_b$ denoting the operator of the boson energy.

3.2.2. Atomic-like motion with spin-dependent localized states at zero temperature

Since $H^{ns}$ depends on boson operators, a certain number of crystal-spin-1 bosons is excited in the ground state of the nonadiabatic Hamiltonian $H^n$ at any temperature. However, at zero temperature we may assume that these bosons are virtually excited, i.e., each boson pair is re-absorbed immediately after its generation, producing in this way an effective electron-electron interaction. Thus, at zero temperature we approximate the nonadiabatic system represented by $H^n$ by a purely electronic system represented by a Hamiltonian

$$H^0 = H_{HF} + H^0_{Cb} \tag{3.5}$$

not depending on boson operators.

Also at zero temperature, the nonadiabatic mechanism specified by Eq. (2.3) occurs in the nonadiabatic system. In the purely electronic system represented by $H^0$, however, the electronic motion is no longer coupled to the motion of the centers of mass of the localized states, but the interaction term $H^0_{Cb}$ of $H^n$ contains the effective electron-electron interaction which is produced by this nonadiabatic mechanism. Thus, the matrix elements of $H^0_{Cb}$ do not follow Eq. (3.2) and the system represented by $H^0$ can be described within the adiabatic approximation. The localized states related to the atomic-like motion now are represented by adiabatic localized func-
tions, i.e., by the spin-dependent Wannier functions
\[ w_{\mathbf{r}m}(\mathbf{r}, t) \equiv w_{\mathbf{r}m}(\mathbf{r} - \mathbf{R} - \mathbf{\rho}_i, t) \] (3.6)
of the superconducting band, as defined in Eq. (A22) of Ref. [1]. The vectors \( \mathbf{T} = \mathbf{R} + \mathbf{\rho}_i \) stand for the positions of the relevant atoms, \( \mathbf{r} \) and \( t \) are the local and spin coordinate, respectively, and \( m \) denotes the quantum number of the crystal spin in the purely electronic system.

Within the nonadiabatic system, the crystal spin is a conserved quantity. Thus, also \( H^0 \) conserves the crystal spin of the localized states,
\[ [H^0, M(\alpha)] = 0 \quad \text{for} \quad \alpha \in G_M. \] (3.7)
The purely electronic system (represented by \( H^0 \)) is not coupled to boson excitations that would be able to store temporarily spin-angular momenta. Hence, \( H^0 \) also conserves the electron spin,
\[ [H^0, S(\alpha)] = 0 \quad \text{for} \quad \alpha \in O(3). \] (3.8)
Consequently, the ground state \( |G^0\rangle \) of \( H^0 \) satisfies the equations
\[ M(\alpha)|G^0\rangle = |G^0\rangle \quad \text{for} \quad \alpha \in G_M \] (3.9)
and
\[ S(\alpha)|G^0\rangle = |G^0\rangle \quad \text{for} \quad \alpha \in O(3). \] (3.10)

In a superconducting band, a randomly chosen \( N \)-electron state will generally not comply with both conditions (3.9) and (3.10) because the Bloch states \( |\mathbf{k}, m\rangle \) with crystal spin \( m \) have \( \mathbf{k} \)-dependent spin directions,
\[ c_{\mathbf{k}qm}^\dagger = \sum_{s=\pm\frac{1}{2}} f_{sm}(q, \mathbf{k}) c_{\mathbf{k}qs}^\dagger. \] (3.11)
The fermion operators \( c_{\mathbf{k}qm}^\dagger \) and \( c_{\mathbf{k}qs}^\dagger \) create Bloch electrons with crystal spin \( m \) and spin \( s \), respectively, and wave vector \( \mathbf{k} \) in the \( q \)-th branch of the superconducting band. The coefficients \( f_{sm}(q, \mathbf{k}) \) determine the direction of the electron spin in the Bloch state \( |\mathbf{k}, m\rangle \) and, consequently, form a unitary two-dimensional matrix depending on \( \mathbf{k} \) and \( q \). In a superconducting band, the matrix \( f_{sm}(q, \mathbf{k}) \) cannot be chosen to be independent of \( \mathbf{k} \). Thus, only very special, if any, \( N \)-electron states comply with both conditions (3.9) and (3.10).

Indeed, there exist states complying with both conditions. Let be \( |G^0\rangle \) a linear combination of states
\[ |\mathbf{p}\rangle = \beta_{\mathbf{k}_1q_1}^\dagger \beta_{\mathbf{k}_2q_2}^\dagger \beta_{\mathbf{k}_3q_3}^\dagger \cdots \beta_{\mathbf{k}_{N/2}q_{N/2}}^\dagger |0\rangle, \] (3.12)
where the new operators
\[ \beta_{\mathbf{k}q}^\dagger = c_{\mathbf{k}qm}^\dagger c_{-\mathbf{k}q-m}^\dagger - c_{\mathbf{k}q-m}^\dagger c_{-\mathbf{k}qm}^\dagger \] (3.13)
create symmetrized Cooper pairs.

From Eq. (3.13) it follows immediately that
\[ M(\alpha)\beta_{\mathbf{k}q}^\dagger M^{-1}(\alpha) = \beta_{\mathbf{k}q}^\dagger \quad \text{for} \quad \alpha \in G_M, \] (3.14)
because the operators \( \beta_{\mathbf{k}q}^\dagger \) form basis functions of the identity representation \( \Gamma_1 \) of \( G_M \). Thus, we have
\[ M(\alpha)|\mathbf{p}\rangle = |\mathbf{p}\rangle \quad \text{for} \quad \alpha \in G_M, \] (3.15)
and hence, Eq. (3.9) is true. Transforming the operators \( \beta_{\mathbf{k}q}^\dagger \) in Eq. (3.13) into the \( s \) representation, we obtain again Cooper pairs of the same form,
\[ \beta_{\mathbf{k}q}^\dagger = c_{\mathbf{k}qs}^\dagger c_{-\mathbf{k}q-s}^\dagger - c_{\mathbf{k}q-s}^\dagger c_{-\mathbf{k}qs}^\dagger, \] (3.16)
demonstrating that also Eq. (3.10) is valid.

Eq. (3.16) can be deduced from Eq. (3.13) using Eq. (3.11) and the time-inversion symmetry of the crystal spin,
\[ Kc_{\mathbf{k}qm}^\dagger K^{-1} = v(m)c_{-\mathbf{k}q-m}^\dagger, \] (3.17)
and of the electron spin,
\[ Kc_{\mathbf{k}qs}^\dagger K^{-1} = v(s)c_{-\mathbf{k}q-s}^\dagger, \] (3.18)
where \( K \) denotes the operator of time inversion and
\[ v(\pm\frac{1}{2}) = \pm 1. \]

The ground state \( |G^0\rangle \) of \( H^0 \) complies with both conditions (3.9) and (3.10) only if the electron forms Cooper pairs invariant under time-inversion. This important result demonstrates that the nonadiabatic spin-boson interaction \( H^0_{\mathbf{C}b} \) in Eq. (3.2) forces the electrons in a novel way to form Cooper pairs below a certain transition temperature. The formation of Cooper pairs is a consequence of the interplay of two conservation laws, namely of the conservation of the electron spin and of the conservation of the crystal spin of the localized states.

### 3.3. Constraining forces required for superconducting eigenstates

To date, it is not possible to solve the Schrödinger equation for the electron-boson system in a solid state. Hence, it cannot be excluded that there exists a condition for superconducting eigenstates not yet considered in the theory of superconductivity.

From the conditions (3.7) and (3.8) it follows that the interaction term of the electronic Hamiltonian \( H^0 \) in Eq. (3.2) has the form
\[ H^0_{\mathbf{C}b} = \sum_{\mathbf{k}q, \mathbf{k}q'} \langle \mathbf{k}, q|H^0_{\mathbf{C}b}|\mathbf{k}', q'\rangle \beta_{\mathbf{k}q}^\dagger \beta_{\mathbf{k}q'}^\dagger, \] (3.19)
showing that \( H^0_{\mathbf{C}b} \) is strongly \( \mathbf{k} \) and \( s \) dependent since
\[ \langle \mathbf{k}_1, s_1; q_1|\mathbf{k}_2, s_2; q_2|H^0_{\mathbf{C}b}|\mathbf{k}_1', s_1'; q_1'|\mathbf{k}_2', s_2'; q_2'\rangle = 0 \] (3.20)
for \( \mathbf{k}_1 \neq -\mathbf{k}_2, \mathbf{k}'_1 \neq -\mathbf{k}'_2, s_1 \neq -s_2 \), or \( s'_1 \neq -s'_2 \).

This Eq. (3.21) may be interpreted as condition of constraint indicating the existence of constraining forces in a narrow superconducting band. Thus, Eq. (3.21) demonstrates that \( H'' \) is acting in a special part of the Hilbert space representing a nonadiabatic system in which constraining forces are effective in a way familiar from classical mechanics. Below a transition temperature, these constraining forces reduce the degrees of freedom of the electron system by forcing the electrons to form pairs that are invariant under time inversion, i.e., by forcing the electrons to form Cooper pairs possessing only half the degrees of freedom of unpaired electrons.

In materials that do not possess a superconducting band, on the other hand, constraining forces halving the degrees of freedom of the electrons do not exist. In the classical mechanics, however, any reduction of the degrees of freedom of any system of particles is caused by constraining forces. Hence, it cannot be excluded that also in quantum mechanical systems any reduction of the electronic degrees of freedom is produced by constraining forces since quantum particles behave in some respects similar to classical particles. This comparison of the quantum system with a classical system suggests that the constraining forces characterized by Eq. (3.21) are required for the formation of Cooper pairs, i.e., they are required for the Hamiltonian to possess superconducting eigenstates. This interpretation is corroborated by the observation that materials not possessing a narrow, partly filled superconducting band do not become superconducting. Thus, the author proposes that materials which do not possess a narrow, partly filled superconducting band, do not become superconducting even if the electrons of the considered material are (weakly or strongly) coupled by an effective electron-electron interaction.

It should be noted that the purely electronic system represented by the Hamiltonian \( H'' \) in Eq. (3.5) only approximates the true nonadiabatic system represented by the operator \( H'' \) given in Eq. (3.4). So, the Cooper pairs are not really rigid as suggested by the ground state \( |G^0 \rangle \) of \( H'' \). In the nonadiabatic system the physics of the mechanism of constraining forces may be demonstrated more realistically in terms of “spring-mounted” Cooper pairs \( ^{17} \).

### 3.4. Calculation of the transition temperature

In accordance with the generally accepted and experimentally corroborated concept of superconductivity, the formation of Cooper pairs is mediated by Boson excitations also within a superconducting band. Further, the constraining forces determined by Eq. (3.21) do not alter the energy of the electron system but only lower the degrees of freedom of the electrons. Consequently, the vast majority of the statements and calculations of the traditional theory of superconductivity should stay valid in a superconducting band. In particular, the superconducting transition temperature \( T_c \) may be calculated also in a superconducting band by a slightly modified BCS equation \( ^{18} \) in the weak-coupling limit \( ^{19} \). A calculation of \( T_c \) within the NHM in the strong-coupling limit remains to be done. Principally, however, the group-theoretical NHM does not provide methods to calculate the matrix elements of \( H''_{CB} \) in Eq. (3.19). Hence, it does not distinguish between weak-coupling and strong-coupling superconductivity. It only proposes that the equation of constraint (3.21) is a universal condition for superconducting eigenstates in the weak-coupling as well as in the strong-coupling limits.

### 4. SUPERCONDUCTING BAND IN MgB$_2$

We show now that the energy band denoted by the bold line is a superconducting band. It is labeled by the representations

\[
\Gamma_5^-, \Gamma_6^+, K_6: M_3, M_2; A_5^+, A_6^-, L_4^+, L_4^-; H_5.
\] (4.1)

Table 1\( ^{19} \) (a) lists all the four bands in MgB$_2$ whose Bloch functions can be unitarily transformed into

| \( \Gamma(000) \), \( A(00\frac{1}{2}) \) | \( E \) | \( C_{2z}^T \) | \( C_{2z}'^T \) | \( C_{4z}^T \) | \( I \) | \( \sigma_h \) | \( \sigma_d \) |
|---|---|---|---|---|---|---|---|
| \( \Gamma_1^T \) | \( A_1^+ \) | 1 | 1 | 1 | 1 | \pm 1 | \pm 1 | \pm 1 | \pm 1 | \pm 1 | \pm 1 |
| \( \Gamma_2^T \) | \( A_2^+ \) | 1 | -1 | 1 | -1 | \pm 1 | \pm 1 | \pm 1 | \pm 1 | \pm 1 | \pm 1 |
| \( \Gamma_3^T \) | \( A_3^+ \) | 1 | 1 | -1 | -1 | \pm 1 | \pm 1 | \mp 1 | \mp 1 | \mp 1 | \mp 1 |
| \( \Gamma_4^T \) | \( A_4^+ \) | 1 | -1 | -1 | 1 | \pm 1 | \pm 1 | \mp 1 | \mp 1 | \mp 1 | \mp 1 |
| \( \Gamma_5^T \) | \( A_5^+ \) | 2 | -1 | 0 | -2 | 0 | \pm 2 | \mp 1 | 0 | \mp 2 | \pm 1 | 0 |
| \( \Gamma_6^T \) | \( A_6^+ \) | 2 | -1 | 0 | 2 | -1 | \pm 2 | \mp 1 | 0 | \mp 2 | \pm 1 | 0 |

| \( M(00\frac{1}{2}) \), \( L(00\frac{1}{2}) \) | \( E \) | \( C_2 \) | \( C_{2z}^T \) | \( C_{2z}'^T \) | \( I \) | \( \sigma_h \) | \( \sigma_d \) | \( \sigma_{d_1} \) |
|---|---|---|---|---|---|---|---|
| \( M_1^T \) | \( L_1^+ \) | 1 | 1 | 1 | 1 | \pm 1 | \pm 1 | \pm 1 | \pm 1 |
| \( M_2^T \) | \( L_2^+ \) | 1 | -1 | 1 | -1 | \pm 1 | \pm 1 | \mp 1 | \mp 1 |
| \( M_3^T \) | \( L_3^+ \) | 1 | -1 | -1 | 1 | \pm 1 | \pm 1 | \mp 1 | \mp 1 |
| \( M_4^T \) | \( L_4^+ \) | 1 | -1 | 1 | \pm 1 | \pm 1 | \mp 1 | \mp 1 |

The band structure of MgB$_2$ is calculated by the two formalisms, one of which is based on the H¹ Hamiltonian, the other on an adiabatic approximation of the H¹ Hamiltonian. The two formalisms are not necessarily equivalent, but they should be identical in the weak-coupling limits.
TABLE II: Character tables of the double-valued irreducible representations of the space group $\Gamma_h D_{6h}^3$ of MgB$_2$, as determined from Table 6.13 of Bradley and Cracknell [10].

| $\Gamma(000), A(00\frac{1}{2})$ | $E$ | $C_2^\pm$ | $C_2'$ | $C_2''$ | $C_{21}'$ | $C_{21}''$ | $C_{21}'''$ |
|-------------------------------|-----|------------|---------|---------|-----------|-----------|-----------|
| $\Gamma^+_7$ $A^+_8$ | 2 | -2 | 0 | 0 | -2 | 0 | 0 | 0 |
| $\Gamma^+_8$ $A^+_8$ | 2 | -2 | $\sqrt{3}$ | $-\sqrt{3}$ | 1 | 1 | 0 | 0 |
| $\Gamma^+_9$ $A^+_8$ | 2 | -2 | $\sqrt{3}$ | $\sqrt{3}$ | 1 | -1 | 0 | 0 |

$\Gamma(000), A(00\frac{1}{2})$ (continued)

| $I$ | $T$ | $S_3^\pm$ | $S_3'$ | $S_3''$ | $S_3'''$ | $S_3''''$ | $S_3'''''$ | $\sigma_h$ | $\sigma_{d_1}$ | $\sigma_{d_2}$ | $\sigma_{d_3}$ | $\sigma_{v_1}$ | $\sigma_{v_2}$ | $\sigma_{v_3}$ | $\sigma_{v_4}$ |
|-----|-----|----------|--------|--------|---------|-----------|----------|--------|--------|--------|--------|--------|--------|--------|--------|
| $\Gamma^+_7$ $A^+_8$ | $\pm2$ | 0 | 0 | $\pm2$ | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| $\Gamma^+_8$ $A^+_8$ | $\pm2$ | $\pm\sqrt{3}$ | $\pm\sqrt{3}$ | $\pm1$ | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| $\Gamma^+_9$ $A^+_8$ | $\pm2$ | $\pm\sqrt{3}$ | $\pm\sqrt{3}$ | $\pm1$ | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

$H(\Gamma^+_7 \pm \frac{1}{2})$, $K(\Gamma^+_8 \pm \frac{1}{2})$

| $E$ | $E$ | $C_2^\pm$ | $C_2'$ | $C_2''$ | $C_{21}'$ | $C_{21}''$ | $C_{21}'''$ | $H_7$ | $K_7$ | $-2$ | $-2$ | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
|-----|-----|------------|---------|---------|-----------|-----------|-----------|--------|--------|---------|--------|---------|--------|---------|--------|---------|--------|---------|--------|---------|--------|---------|--------|---------|
| $H_8$ | $K_8$ | 2 | -2 | $\sqrt{3}$ | $-\sqrt{3}$ | 1 | 1 | 0 | 0 | 0 | 0 | 0 |
| $H_9$ | $K_9$ | 2 | -2 | $-\sqrt{3}$ | $\sqrt{3}$ | 1 | -1 | 0 | 0 | 0 | 0 | 0 |

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

| $C_2'$ | $C_{21}'$ | $C_{21}''$ | $C_{21}'''$ | $\sigma_h$ | $\sigma_{d_1}$ | $\sigma_{d_2}$ | $\sigma_{v_1}$ | $\sigma_{v_2}$ | $\sigma_{v_3}$ | $\sigma_{v_4}$ |
|-------|------------|-----------|-----------|--------|--------|--------|--------|--------|--------|--------|
| $E$ | $E$ | $C_2'$ | $C_{21}'$ | $C_{21}''$ | $C_{21}'''$ | $\sigma_h$ | $\sigma_{d_1}$ | $\sigma_{d_2}$ | $\sigma_{v_1}$ | $\sigma_{v_2}$ | $\sigma_{v_3}$ | $\sigma_{v_4}$ |
| $M^+_7$ | $L^+_7$ | 2 | -2 | 0 | 0 | $\pm2$ | $\pm2$ | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

TABLE III: Compatibility relations between the single-valued (upper row) and double-valued (lower row) representations of the space group $\Gamma_h D_{6h}^3$ of MgB$_2$.

| $\Gamma, A$ | $L, M$ |
|-------------|--------|
| $R^+_7$, $R^+_8$, $R^+_9$, $R^+_{10}$, $R^+_{11}$, $R^+_{12}$ | $R^+_6$ |
| $R^+_7$, $R^+_8$, $R^+_9$, $R^+_{10}$, $R^+_{11}$, $R^+_{12}$ | $R^+_6$ |

Notes to Table III

(i) The single-valued and double-valued representations are listed in Tables II and III, respectively.

(ii) Each column lists the double-valued representation $R_i \times D_{1/2}$ below the single-valued representation $R_i$.

These Wannier functions are only weakly spin dependent since they do not strongly differ from the Wannier function belonging to band 4 in Table IV (a). It is only the representations $\Gamma^+_7 + \Gamma^+_8$ and $A^+_7 + A^+_8$ of band 4 in Table IV (a) which do not belong to the representations $\Lambda.11.1$. Between A and L the superconducting band jumps from the upper to the lower band. This small jump is allowed within the NHM because the Bloch functions of both bands belong to the same double-valued representation and the jump does not cross the Fermi level.

5. DISCUSSION

This paper shows that the intermetallic superconducting compound MgB$_2$ possesses a narrow, roughly half-filled “superconducting band” in its band structure, see Fig. 1. In addition to the previous observations about elemental superconductors, non-superconductors, YBa$_2$Cu$_3$O$_7$, and La$_2$CuO$_4$ (as mentioned in Sec. I) this result provides further evidence that superconducting bands are a general feature of both weak-coupling and strong-coupling superconductors. Hence, the author proposes that in any material Cooper pairs are stabilized by the constraining forces determined by the condition of constraint (3.20) and generated by the nonadiabatic condensation mechanism characterized by Eq. (2.3). These constraining forces are effective only in narrow superconducting bands and are proposed to be required that the Hamiltonian of the electron-boson system possesses superconducting eigenstates.

The symmetry of the Bloch functions of the entire superconducting band determines the symmetry and spin dependence of the nonadiabatic localized states. The nonadiabatic condensation mechanism characterized by Eq. (2.3), on the other hand, is produced by the Coulomb correlation energy of the electrons near the Fermi level,
TABLE IV: Single- and double-valued representations of all the energy bands in MgB$_2$ with symmetry-adapted and optimally localized (spin-dependent) Wannier functions centered at the B atoms.

(a) Single-valued representations

| Band 1 | Γ$_2$ + Γ$_3$ | L$_2$ + L$_3$ | M$_1$ + M$_2$ | A$_1$ + A$_2$ | K$_5$ | H$_6$ |
| Band 2 | Γ$_2$ + Γ$_3$ | L$_2$ + L$_3$ | M$_1$ + M$_2$ | A$_1$ + A$_2$ | K$_5$ | H$_6$ |
| Band 3 | Γ$_3$ + Γ$_1$ | L$_2$ + L$_3$ | M$_1$ + M$_2$ | A$_1$ + A$_2$ | K$_6$ | H$_5$ |

(b) Double-valued representations

| Γ | M | A |
|---|---|---|
| Band 1 | Γ$_2$ + Γ$_3$ | L$_2$ + L$_3$ | M$_1$ + M$_2$ | A$_1$ + A$_2$ |
| Band 2 | Γ$_2$ + Γ$_3$ | L$_2$ + L$_3$ | M$_1$ + M$_2$ | A$_1$ + A$_2$ |
| Band 3 | Γ$_3$ + Γ$_1$ | L$_2$ + L$_3$ | M$_1$ + M$_2$ | A$_1$ + A$_2$ |

Notes to Table IV

(i) The bands 2 and 3 in Table IV(b) form superconducting bands.

(ii) Band 1 of Table IV(b) is not a superconducting band because the representations Γ$_2$ and Γ$_3$ cannot be written in the form $R \times D_{1/2}$ where $R$ stands for any one-dimensional single-valued representation and $D_{1/2}$ denotes the two-dimensional double-valued representation of the three-dimensional rotation group $O(3)$. The form $R \times D_{1/2}$ of the representations Γ$_2$ and Γ$_3$ belonging to bands 2 and 3 in Table IV(b) ensures that the spin-dependent Wannier functions transform under the space group operations like spin functions, see Eq. (28) of Ref. [1].

(iii) The single-valued and double-valued representations are listed in Tables III and II, respectively.

(iv) Each row defines one band consisting of two branches, because there are two B atoms in the unit cell.

(v) The bands are determined by Eq. (23) of Ref. [7].

(vi) Assume a band of the symmetry in any row of this table to exist in the band structure of MgB$_2$. Then Bloch functions of this band can be unitarily transformed into Wannier functions that are

- localized as well as possible;
- centered at the B atoms; and
- symmetry-adapted to the space group $\Gamma h D_{1/2}$ of MgB$_2$.

These Wannier function are usual (spin-independent) Wannier function if the considered band is characterized by the single-valued representations (a). They are spin dependent if the band is characterized by the double-valued representations (b).

in accordance with the generally accepted concept that correlated conduction electrons are responsible for superconductivity.

Further, in accordance with the general belief, also in superconducting bands the formation of Cooper pairs is mediated by boson excitations. In superconducting bands, however, the pair formation is mediated by the energetically lowest boson excitations of the crystal that possess the crystal-spin angular momentum $l \cdot h$ and are sufficiently stable to transport it through the crystal. These "crystal-spin" bosons are localized excitations $|T, l\rangle$ (with $l = -1, 0, +1$ labeling the three directions of the crystal spin and $T$ denoting a lattice point) of well-defined symmetry [14, 20] which propagate as Bloch waves (with the crystal momentum $h \cdot k$) through the crystal.

The $|T, l\rangle$ are generated during spin-flip processes in the superconducting band and must carry off the surplus crystal-spin angular-momenta generated at these processes. This spin-boson mechanism suggests that the $|T, l\rangle$ are coupled phonon-plasmon modes: In a first step the atomic-like electrons in the superconducting band transmit their angular momenta to the core electrons by generating a plasmon-like vibration of the core electrons against the atoms. In a second step, these plasmon-like excitations generate phonon-like vibrations of lower energy if crystal-spin-1 phonons are sufficiently stable in the considered material.

Thus, the author proposes that the $|T, l\rangle$ are coupled phonon-plasmon modes which have dominant phonon character in the isotropic lattices of the transition elements and, hence, confirm the electron-phonon mechanism that enters the BCS theory [18] in these materials [13]. However, phonon-like excitations are not able to transport crystal-spin angular-momenta within the two-dimensional copper-oxygen layers of the cuprates, see Ref. [20] for preliminary ideas to this problem. Within two-dimensional layers, the $|T, l\rangle$ necessarily are energetically higher lying excitations of dominant plasmon character. This clear dependence of stable crystal-spin-1 bosons on the properties of the lattice suggests that they are (at least partially) responsible for the special properties of the layered superconductors, i.e., their strong-coupling features and their high transition temperatures.

Also MgB$_2$ contains two-dimensional hexagonal nets of B atoms. Thus, also in this layered material crystal-spin-1 phonons will be less stable than in the isotropic lattices of the transition elements. The balance between the phonon and plasmon character of stable crystal-spin-1 excitations is shifted towards the plasmon character leading to a higher transition temperature and to the experimentally established [21, 22, 23] reduced isotope effect.

The superconducting band in MgB$_2$ is composed of $\sigma$- and $\pi$-bands in accordance with the two-band model of superconductivity [24, 25] in this material characterized by $\sigma$- and $\pi$-bands associated with different parts of the Fermi surface [26]. The part of the Fermi surface of the
superconducting band enclosing the points Γ and A has σ character, the other parts have π character.

In the band structures of the two-dimensional superconductors YBa$_2$Cu$_3$O$_7$ [10], MgB$_2$ (this paper), and La$_2$CuO$_4$ [11] I found a new feature of the superconducting bands: the related spin-dependent Wannier functions are only weakly spin dependent. I believe that this weak spin dependence is an additional condition for stable two-dimensional high-$T_c$ superconducting states. This question requires further theoretical consideration and further examination of the band structures of high-$T_c$ superconductors.

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