Helical magnetic ordering and superconductivity in $HoNi_2B_2C$

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The effect of helicoidal magnetic ordering on superconductivity in $HoNi_2B_2C$ and the character of superconducting pairing in the helicoidal phase have been studied. The analysis leads to the conclusion that the strong suppression of superconductivity in the helicoidal phase region results from a significant modification of electron wave functions owing to crossings of the Fermi surface corresponding to the paramagnetic phase by Bragg planes resulting from the helicoidal ordering. The decoupling effect of nonmagnetic impurities in the region in which superconductivity and antiferromagnetism coexist remains unsaturated, increases as the impurity concentration. © *1996 American Institute of Physics.* [S1063-7761(96)02511-5]

1. INTRODUCTION

After the discovery in 1994 of superconducting borocarbides $ReNi_2B_2C$, where Re is a rare-earth element, in which antiferromagnetic ordering takes place in the superconducting state, researchers' attention has been again attracted to the problem of coexistence of superconductivity and magnetism.

This problem aroused general interest for the first time in the late 1970s owing to the discovery of $ReRh_4B_4$ and $ReMo_6S_8$ compounds, in which both magnetic ordering and superconductivity were detected. A thorough examination of these compounds allowed the researchers to detect and describe many effects of interaction between the superconducting and magnetic order parameters. The main results of this research were reported in Ref. 1.

The most interesting effect attracting the researchers' attention is the reentrant (or almost reentrant) behavior of superconductivity in $HoNi_2B_2C$, which belongs to the class of borocarbides.

Earlier, reentrant superconductivity was detected in $ErRh_4B_4$ and $HoMo_6S_8$. In those compounds it was due to ferromagnetic ordering at temperatures below T_m, which is lower than the superconducting transition temperature T_c. The effect of superconducting ordering on the magnetic subsystem leads to cryptomagnetism,[2] i.e., in a temperature range of about 0.05 K around T_m, superconductivity coexists with long-wave antiferromagnetic order whose wavelength is controlled by the superconducting gap in the electronic quasiparticle spectrum. At lower temperatures superconductivity is destroyed, and the sample transforms to a normal ferromagnetic state via a first-order phase transition (see, for example, Ref. 1).

If the superconducting transition temperature T_c was below that of antiferromagnetic ordering, which is the case in $ReMo_6S_8$ (Re = Tb, Dy) and $ReRh_4B_4$ (Re = Nb, Sm, Tm), superconductivity was not destroyed.

In $HoNi_2B_2C$, reentrant[3–5] or almost reentrant[6,7] superconductivity was detected over a narrow range of incommensurate helicoidal magnetic ordering. This ordering emerged at $T_m=5.7$–6.0 K, which is below $T_c=8.1$ K. At $T_N=5.2$ K, a first-order phase transition to a phase with a commensurate antiferromagnetic order occurred.[7]

The suppression of superconductivity, manifested by a decrease in the critical field H_{c2}, occurred at temperatures below T_m. In some specimens the final result was a transition to the normal phase at a temperature T_{c2} ($T_N<T_{c2}<T_m$)[3–5], in others the superconductivity survived, although it degraded considerably, in the temperature range down to T_N. The transition to the commensurate phase coincided with the restoration of the superconducting order parameter, and then it increased to a value higher than at T_m (Fig. 1). There was no jump in H_{c2} at T_N because the helicoidal and commensurate phases coexisted over a certain temperature range.[8]

Neutron diffraction data indicate that the wave vector of helicoidal magnetic order is constant over its entire range of existence, and is insensitive to the destruction of superconductivity.[3,8–10] Hence the observed magnetic ordering bears no relation to cryptomagnetism.

In a previous publication,[11] it was suggested that the strong effect of magnetic ordering on superconductivity in $HoNi_2B_2C$ results from newly emergent magnetic Bragg planes crossing the Fermi surface of electrons in the paramagnetic phase, while differences in the degree of superconductivity suppression are due to differences in nonmagnetic impurity concentrations. One goal of the present paper is to examine this issue in detail.

Since helicoidal magnetic ordering modifies wave functions of conducting electrons and lifts the spin degeneracy of their spectrum, a question arises about anomalous means corresponding to superconducting pairs in the helicoidal phase. Various views on this issue have been reported in the literature. The primary aim of the present paper is to dispose of these inconsistencies and unambiguously determine the nature of superconducting pairing in the helicoidal phase.

In addition, we consider the effect of nonmagnetic impurities on superconductivity near T_m. It is known[12] that nonmagnetic impurities suppress superconductivity in the presence of antiferromagnetic order. According to Ref. 13, near the point of the antiferromagnetic second-order transition, when the magnetic order parameter is small, the effect

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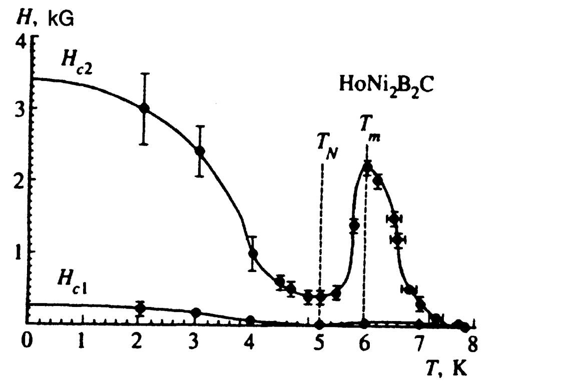

FIG. 1. Critical magnetic fields in $HoNi_2B_2C$ as a function of temperature.[7]

of nonmagnetic impurities becomes independent of their concentration, i.e. this effect is saturated.

We demonstrate below that saturation does not take place, and that the degree of superconductivity suppression by nonmagmetic impurities grows with impurity concentration both near and far from T_m.

Section 2 describes modified wave functions and spectra of electrons in the helicoidal phase. Section 3 considers the issue of anomalous means in the helicoidal phase of a pure superconductor. In Sec. 4 we discuss the effect of nonmagnetic impurities on superconductivity. Section 5 summarizes the main results.

2. EFFECT OF HELICOIDAL MAGNETIC ORDER ON ELECTRONIC SPECTRUM

At $T>T_m$ the compound $HoNi_2B_2C$ is in a paramagnetic phase with a tetragonal body-centered Bravais lattice (Fig. 2). The rare-earth ions form layers perpendicular to the fourth-order c axis.

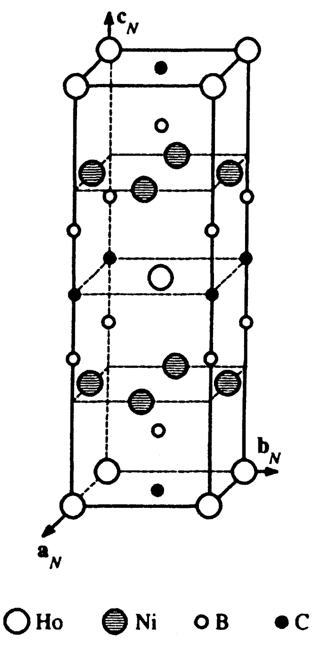

FIG. 2. Elementary cell of $HoNi_2B_2C$.

At $T<T_N$ the elementary cell of $HoNi_2B_2C$ is doubled since the magnetic moments of Ho in the layers are ferromagnetically ordered in the [100] direction, and magnetizations of neighboring layers are aligned in opposite directions. The Bravais lattice becomes primitive tetragonal. We denote the elementary vectors of the reciprocal lattice of this phase as $\mathbf{a}^*$, $\mathbf{b}^*$, and $\mathbf{c}^*$. Antiferromagnetic order in the commensurate phase is then characterized by the vector $\mathbf{c}^*$.

In the helicoidal phase of $HoNi_2B_2C$, the holmium magnetic moments are still aligned in the ab plane, but their direction is variable in the directions of both the a and c axes. The corresponding magnetic order wave vector $\mathbf{Q}$ is[8,9]

$$\mathbf{Q}=0.585\mathbf{a}^*+0.913\mathbf{c}^*. \tag{1}$$

The distinction between the magnetic order vectors in the commensurate and incommensurate phases results in a radical difference between the effects of magnetic order on superconductivity in these phases.

The average holmium spin at a point with coordinates $\mathbf{R}_k$ in the helicoidal phase is

$$\mathbf{S}(\mathbf{R}_k)=\mathbf{i}S\cos(\mathbf{Q}\mathbf{R}_k)+\mathbf{j}S\sin(\mathbf{Q}\mathbf{R}_k), \tag{2}$$

where S is the average ion spin, and $\mathbf{i}$ and $\mathbf{j}$ are unit vectors aligned with the a and b axes, respectively.

The Hamiltonian of conduction electrons, taking into account the $s-f$ exchange interaction with the mean ionic holmium spins, has the form

$$\mathscr{H}_e=\sum_{\mathbf{k},\alpha,\beta}\Big\{\varepsilon(\mathbf{k})\delta_{\alpha\beta}a_\alpha^+(\mathbf{k})a_\beta(\mathbf{k}) +\frac{1}{2}I_{s-f}S[a_\alpha^+(\mathbf{k}-\mathbf{Q})\sigma_{\alpha\beta}^+a_\beta(\mathbf{k}) +a_\alpha^+(\mathbf{k}+\mathbf{Q})\sigma_{\alpha\beta}^-a_\beta(\mathbf{k})]\Big\}. \tag{3}$$

Here $\varepsilon(\mathbf{k})$, $a_\alpha^+(\mathbf{k})$, and $a_\alpha(\mathbf{k})$ are the dispersion relation and second quantization operators for electrons in the paramagnetic phase, I_{s-f} is the integral of the $s-f$ exchange interaction, $\alpha,\ \beta=1,\ 2$ correspond to the electron-spin projections on the c axis $(+1/2$ and $-1/2)$, and $\sigma^{\pm}=\sigma_x\pm i\sigma_y$ (σ_x and σ_y are Pauli matrices).

Helicoidal magnetic order mixes states with different spin projections on the c axis, lifts the spin degeneracy of the electron spectrum, and generates new Bragg planes, which differ among the resulting dispersion relations.[14]

The Hamiltonian (3) can be diagonalized in the representation of the new electron states described by the wave functions

$$\tilde{\psi}_{1,\mathbf{k}}(\mathbf{r})=u(\mathbf{k})\psi_{1,\mathbf{k}}(\mathbf{r})+v(\mathbf{k})\psi_{2,\mathbf{k}+\mathbf{Q}}(\mathbf{r}), \tag{4}$$

$$\tilde{\psi}_{2,\mathbf{k}}(\mathbf{r})=u(-\mathbf{k})\psi_{2,\mathbf{k}}(\mathbf{r})+v(-\mathbf{k})\psi_{1,\mathbf{k}-\mathbf{Q}}(\mathbf{r}), \tag{5}$$

where $\psi_{\alpha,\mathbf{k}}(\mathbf{r})$ are Bloch functions in the paramagnetic phase (α is the spin index),

$$u(\mathbf{k})=\sqrt{\frac{1}{2}\left[1+\sqrt{\frac{[\varepsilon(\mathbf{k})-\varepsilon(\mathbf{k}+\mathbf{Q})]^2}{[\varepsilon(\mathbf{k})-\varepsilon(\mathbf{k}+\mathbf{Q})]^2+I_{s-f}^2S^2}}\right]}, \tag{6}$$

$$v(\mathbf{k})=\pm\sqrt{1-u^2(\mathbf{k})}. \tag{7}$$

The corresponding dispersion relations are:

$$\tilde{\varepsilon}_1(\mathbf{k})=\frac{1}{2}\{\varepsilon(\mathbf{k})+\varepsilon(\mathbf{k}+\mathbf{Q})\pm[(\varepsilon(\mathbf{k})-\varepsilon(\mathbf{k}+\mathbf{Q}))^2+I_{s-f}^2S^2]^{1/2}\}, \tag{8}$$

$$\tilde{\varepsilon}_2(\mathbf{k})=\frac{1}{2}\{\varepsilon(\mathbf{k})+\varepsilon(\mathbf{k}-\mathbf{Q})\pm[(\varepsilon(\mathbf{k})-\varepsilon(\mathbf{k}-\mathbf{Q}))^2+I_{s-f}^2S^2]^{1/2}\} \tag{9}$$

with discontinuities corresponding to wave vectors $\mathbf{g}_i+\mathbf{Q}$ and $\mathbf{g}_i-\mathbf{Q}$, respectively ($\mathbf{g}_i$ is the reciprocal lattice vector in the paramagnetic phase, and $\varepsilon(\mathbf{k})=\varepsilon(\mathbf{k}+\mathbf{g}_i)$). The signs in Eqs. (7)–(9) are selected so as to obtain the original dispersion relation in the limit $S\to 0$.

In the commensurate phase, the antiferromagnetic order vector is half of one of reciprocal lattice vectors of the paramagnetic phase ($\mathbf{c}^*=\mathbf{g}_0/2$), so the electron dispersion relation remains spin degenerate.

Since the magnetization is modulated in the direction of the a axis in the incommensurate phase, the locations of the Bragg planes in the incommensurate and commensurate phases are radically different.

3. SUPERCONDUCTIVITY IN THE CASE OF HELICOIDAL MAGNETIC ORDER

We now examine the effect of helicoidal magnetic order on superconductivity resulting from electron–phonon coupling. Since T_c is of the order of T_m, the superconducting energy per elementary cell $\sim T_c^2/\varepsilon_F$, where ε_F is the electron Fermi energy, is much less than the corresponding magnetic energy $\sim T_m$, and the back influence of superconductivity on magnetic order is negligible.

The magnetic subsystem affects superconductivity in three ways:

1. repulsion between electrons in the s-channel due to their interaction via spin fluctuations;

2. modification of electron wave functions due to the emergence of new Bragg planes generated by magnetic order. This effect changes matrix elements of the electron–phonon interaction and the electron density of states at the Fermi surface;

3. decoupling action of nonmagnetic impurities in the region where superconductivity and antiferromagnetism coexist, which is also due to the modification of electron wave functions and resulting violation of the Anderson theorem.

If the first of these factors were the most important, the suppression of superconductivity would be the strongest at $T=T_m$, where spin fluctuations are most intense, the superconducting order parameter, if interactions with the magnetic system are neglected, is not so high as at $T<T_m$. But the suppression of superconductivity is strongest (provided that it survives) in the incommensurate phase at $T\to T_M$ (Fig. 1). In materials where superconductivity is destroyed, this happens at $T_{c2}<T_m$.[3–5]

We therefore conclude that the second and third factors are the most important. But they are also active in the commensurate phase. A natural question arises: why is their effect not so strong in the commensurate phase?

We start with a simple model in which the electron–phonon interaction in the paramagnetic phase is described by the Hamiltonian

$$\mathscr{H}_{\mathrm{e-ph}}=g_{\mathrm{ph}}\sum_{\mathbf{k},\mathbf{k}',\alpha} a_\alpha^+(\mathbf{k}')a_\alpha(\mathbf{k})[b^+(\mathbf{k}-\mathbf{k}')+b(\mathbf{k}'-\mathbf{k})], \tag{10}$$

where $g_{\mathrm{ph}}=\mathrm{const}$, and $b^+(\mathbf{q})$ and $b(\mathbf{q})$ are second quantization operators for phonons. For simplicity we consider only one phonon branch.

Since the Eliashberg equations contain screened matrix elements of the electron–phonon interaction, which have no singularities at small transmitted wave vectors, this approximation describes the actual situation fairly well.

By expressing $a_\alpha^+(\mathbf{k})$ and $a_\alpha(\mathbf{k})$ in terms of the new creation, and annihilation, operators $\tilde{a}_\alpha^+(\mathbf{k})$ and $\tilde{a}_\alpha(\mathbf{k})$ which are related to the wave functions (4) and (5), we obtain an expression for $\mathscr{H}_{\mathrm{e-ph}}$ in the magnetically ordered phase:

$$\begin{aligned}\mathscr{H}_{\mathrm{e-ph}}=g_{\mathrm{ph}}\sum_{\mathbf{k},\mathbf{k}'}\{&[u(\mathbf{k})u(\mathbf{k}')+v(\mathbf{k})v(\mathbf{k}')]\tilde{a}_1^+(\mathbf{k}')\tilde{a}_1(\mathbf{k})\\&\times[b^+(\mathbf{k}-\mathbf{k}')+b(\mathbf{k}'-\mathbf{k})]+[u(-\mathbf{k})u(-\mathbf{k}')\\&+v(-\mathbf{k})v(-\mathbf{k}')]\tilde{a}_2^+(\mathbf{k}')\tilde{a}_2(\mathbf{k})[b^+(\mathbf{k}-\mathbf{k}')\\&+b(\mathbf{k}'-\mathbf{k})]+[u(\mathbf{k}')v(-\mathbf{k})+v(\mathbf{k}')u(-\mathbf{k})]\\&\times\tilde{a}_1^+(\mathbf{k}')\tilde{a}_2(\mathbf{k})[b^+(\mathbf{k}-\mathbf{k}'-\mathbf{Q})+b(\mathbf{k}'-\mathbf{k}+\mathbf{Q})]\\&+[u(\mathbf{k})v(-\mathbf{k}')+v(\mathbf{k})u(-\mathbf{k}')]\tilde{a}_2^+(\mathbf{k}')\tilde{a}_1(\mathbf{k})\\&\times[b^+(\mathbf{k}-\mathbf{k}'+\mathbf{Q})+b(\mathbf{k}'-\mathbf{k}-\mathbf{Q})].\end{aligned} \tag{11}$$

We assume that conventional s-type singlet coupling takes place in the paramagnetic phase. In the helicoidal phase, generally speaking, anomalous means like both $\langle\tilde{a}_i^+(-\mathbf{k})\tilde{a}_i^+(\mathbf{k})\rangle$ $(i=1,2)$ and $\langle\tilde{a}_2^+(-\mathbf{k})\tilde{a}_1^+(\mathbf{k})\rangle$, as well as their linear combinations, can occur. We denote the superconducting order parameter corresponding to the first type of anomalous means as Δ_{ii} and that corresponding to the second type as Δ_{21}.

We now consider the self-consistency equations for them in the weak-coupling approximation:

$$\begin{aligned}\Delta_{11}(\mathbf{k},\varepsilon_k)=-\frac{\pi T}{\Omega}\sum_{\varepsilon_l}\Bigg\{&\int\frac{d^2\mathbf{k}'d\xi_1}{(2\pi)^3|\nabla\tilde{\varepsilon}_1(\mathbf{k}')|}[\Gamma_{11}(-\mathbf{k}',\\&-\mathbf{k})F_{11}^+(\mathbf{k}',\varepsilon_l)\Gamma_{11}(\mathbf{k}',\mathbf{k})D(\mathbf{k}-\mathbf{k}',\varepsilon_k-\varepsilon_l)]\\&+\int\frac{d^2\mathbf{k}'d\xi_2}{(2\pi)^3|\nabla\tilde{\varepsilon}_2(\mathbf{k}')|}[\Gamma_{21}(-\mathbf{k}',-\mathbf{k})\\&\times F_{22}^+(\mathbf{k}',\varepsilon_l)\Gamma_{21}(\mathbf{k}',\mathbf{k})D(\mathbf{k}-\mathbf{k}'-\mathbf{Q},\varepsilon_k-\varepsilon_l)]\Bigg\},\end{aligned} \tag{12}$$

$$\Delta_{21}(\mathbf{k},\varepsilon_k)=-\frac{\pi T}{\Omega}\sum_{\varepsilon_l}\Bigg\{\int\frac{d^2\mathbf{k}'d\xi_1}{(2\pi)^3|\nabla\tilde{\varepsilon}_1(\mathbf{k}')|}[\Gamma_{22}(-\mathbf{k}',$$

$$-\mathbf{k})F_{21}^{+}(\mathbf{k}',\varepsilon_l)\times\Gamma_{11}(\mathbf{k}',\mathbf{k})D(\mathbf{k}-\mathbf{k}',\varepsilon_k-\varepsilon_l)]+\int\frac{d^2\mathbf{k}'d\xi_2}{(2\pi)^3|\nabla\tilde{\varepsilon}_2(\mathbf{k}')|}[\Gamma_{12}(-\mathbf{k}',-\mathbf{k})\times F_{12}^{+}(\mathbf{k}',\varepsilon_l)\Gamma_{21}(\mathbf{k}',\mathbf{k})D(\mathbf{k}-\mathbf{k}'-\mathbf{Q},\varepsilon_k-\varepsilon_l)]\Bigg\},\quad(13)$$

where Ω is the elementary cell volume, ε_k and ε_l are Matsubara frequencies, and $\xi_i=\tilde{\varepsilon}_i(\mathbf{k}')-\mu$ (μ is the chemical potential of electrons). The integration over $d\mathbf{k}'$ is performed over one of the parts of the Fermi surface resulting from the intersection of the appropriate dispersion relation and the Fermi level; the $F_{ij}^{+}(\mathbf{k},\varepsilon_l)$ are anomalous electron Green's functions. The matrix elements $\Gamma_{ij}(\mathbf{k}',\mathbf{k})$ of the electron–phonon interaction, according to Eq. (11), are

$$\Gamma_{11}(\mathbf{k},\mathbf{k}')=g_{\text{ph}}[u(\mathbf{k})u(\mathbf{k}')+v(\mathbf{k})v(\mathbf{k}')],\quad(14)$$

$$\Gamma_{22}(\mathbf{k},\mathbf{k}')=g_{\text{ph}}[u(-\mathbf{k})u(-\mathbf{k}')+v(-\mathbf{k})v(-\mathbf{k}')],\quad(15)$$

$$\Gamma_{12}(\mathbf{k},\mathbf{k}')=g_{\text{ph}}[u(\mathbf{k})v(-\mathbf{k}')+v(\mathbf{k})u(-\mathbf{k}')],\quad(16)$$

$$\Gamma_{21}(\mathbf{k},\mathbf{k}')=g_{\text{ph}}[v(-\mathbf{k})u(\mathbf{k}')+u(-\mathbf{k})v(\mathbf{k}')].\quad(17)$$

The phonon Green's function $D(\mathbf{q},\varepsilon_k-\varepsilon_l)$ in our approximation is

$$D(\mathbf{q},\varepsilon_k-\varepsilon_l)=-\frac{\omega_c^2}{\omega_c^2+(\varepsilon_k-\varepsilon_l)^2},\quad(18)$$

where ω_c is the characteristic phonon frequency.

For simplicity the terms due to direct Coulomb interaction and interaction via spin fluctuations are omitted in Eqs. (12) and (13).

The normal, $G_{ij}(\mathbf{k},\varepsilon_l)$, and anomalous, $F_{ij}^{+}(\mathbf{k},\varepsilon_l)$, electron Green's functions are derived from the following Gor'kov equations:

$$G_{11}(\mathbf{k},\varepsilon_k)=G_{11}^{0}(\mathbf{k},\varepsilon_k)[1+\Delta_{11}^{*}(\mathbf{k},\varepsilon_k)F_{11}^{+}(\mathbf{k},\varepsilon_k)+\Delta_{12}^{*}(\mathbf{k},\varepsilon_k)F_{21}^{+}(\mathbf{k},\varepsilon_k)],\quad(19)$$

$$F_{11}^{+}(\mathbf{k},\varepsilon_k)=G_{11}^{0}(-\mathbf{k},-\varepsilon_k)[\Delta_{11}(\mathbf{k},\varepsilon_k)G_{11}(\mathbf{k},\varepsilon_k)+\Delta_{12}(\mathbf{k},\varepsilon_k)G_{21}(\mathbf{k},\varepsilon_k)],\quad(20)$$

$$G_{21}(\mathbf{k},\varepsilon_k)=G_{22}^{0}(\mathbf{k},\varepsilon_k)[\Delta_{22}^{*}(\mathbf{k},\varepsilon_k)F_{21}^{+}(\mathbf{k},\varepsilon_k)+\Delta_{21}^{*}(\mathbf{k},\varepsilon_k)F_{11}^{+}(\mathbf{k},\varepsilon_k)],\quad(21)$$

$$F_{21}^{+}(\mathbf{k},\varepsilon_k)=G_{22}^{0}(-\mathbf{k},-\varepsilon_k)[\Delta_{21}(\mathbf{k},\varepsilon_k)G_{11}(\mathbf{k},\varepsilon_k)+\Delta_{22}(\mathbf{k},\varepsilon_k)G_{21}(\mathbf{k},\varepsilon_k)].\quad(22)$$

Here $G_{ii}^{0}(\mathbf{k},\varepsilon_k)$ are bare normal electron Green's functions:

$$G_{ii}^{0}(\mathbf{k},\varepsilon_k)=[i\varepsilon_k-\xi_i]^{-1}.\quad(23)$$

An analysis of Eqs. (12), (13), and (19)–(22) shows that there is no linear relation between Δ_{ii} and Δ_{21}, i.e., if one of these parameters is nonzero, it does not automatically mean that the other is also nonzero. Since Δ_{21} transforms to the order parameter corresponding to the common singlet pairing in the paramagnetic phase as $T\to T_m$, it cannot vanish abruptly below T_m, since the parameter S is small near T_m.

At the same time, Δ_{ii} transforms to the order parameter corresponding to triplet pairing in the paramagnetic phase as $T\to T_m$. Since we have assumed that the pairing in the paramagnetic phase is singlet, the temperature T_m can coincide with the temperature at which superconducting pairing occurs with an order parameter like Δ_{ii} only accidentally. Thus there is no reason to suppose that Δ_{ii} is nonzero at temperatures below T_m.

We now consider the conditions for pairing of this type, assuming that Δ_{ii} is a vanishing parameter. We then derive the following well-known expressions from Eqs. (19)–(22):

$$G_{11}(\mathbf{k},\varepsilon_k)=-\frac{i\varepsilon_k+\xi_1}{\varepsilon_k^2+\xi_1^2+\Delta_{21}^2(\mathbf{k},\varepsilon_k)},\quad(24)$$

$$F_{21}^{+}(\mathbf{k},\varepsilon_k)=\frac{\Delta_{21}(\mathbf{k},\varepsilon_k)}{\varepsilon_k^2+\xi_1^2+\Delta_{21}^2(\mathbf{k},\varepsilon_k)},\quad(25)$$

along with

$$F_{ii}^{+}(\mathbf{k},\varepsilon_k)=G_{ii}(-\mathbf{k},-\varepsilon_k)\Delta_{ii}(\mathbf{k},\varepsilon_k)G_{ii}(\mathbf{k},\varepsilon_k).\quad(26)$$

After substituting Eq. (26) into the self-consistency equation (12), one can easily prove that the presence of the superconducting order parameter Δ_{21} makes the existence of Δ_{ii} less likely, since it leads to a cutoff in the lower logarithmic divergence in the sum over ε_l.

As the magnetic order parameter S increases, the splitting $|\tilde{\varepsilon}_i(\mathbf{k})-\tilde{\varepsilon}_i(-\mathbf{k})|$ widens, which makes the emergence of nonzero Δ_{ii} even less likely, since this splitting has the same effect on this type of pairing that ferromagnetic splitting of the dispersion relations of electrons with opposite spins has on the usual singlet pairing.

We conclude that the pairing in the helicoidal phase is of the $\langle\tilde{a}_2^{+}(-\mathbf{k})\tilde{a}_1^{+}(\mathbf{k})\rangle$ type. Bulaevskiĭ *et al.*,[15] who considered the superconducting pairing in terms of the BCS theory, suggested that in the helicoidal phase near T_m the anomalous means have the form $\langle a_2^{+}(-\mathbf{k})a_1^{+}(\mathbf{k})\rangle$, where $a_i^{+}(\mathbf{k})$ are electron creation operators in the paramagnetic phase. If the $a_i^{+}(\mathbf{k})$ are expressed in terms of the modified creation operators $\tilde{a}_i^{+}(\mathbf{k})$ according to Eqs. (4) and (5), it turns out that this coupling corresponds to a superposition of anomalous means like $\langle\tilde{a}_i^{+}(-\mathbf{k})\tilde{a}_i^{+}(\mathbf{k})\rangle$ and $\langle\tilde{a}_2^{+}(-\mathbf{k})\tilde{a}_1^{+}(\mathbf{k})\rangle$. As was demonstrated above, this kind of coupling does not occur.

Note that in the helicoidal phase $\tilde{\varepsilon}_i(\mathbf{k})\neq\tilde{\varepsilon}_i(-\mathbf{k})$, and coupling modes like both $\langle\tilde{a}_i^{+}(-\mathbf{k})\tilde{a}_i^{+}(\mathbf{k})\rangle$ and $\langle\tilde{a}_2^{+}(-\mathbf{k})\tilde{a}_1^{+}(\mathbf{k})\rangle$ are neither purely triplet nor purely singlet ($|\Delta_{ij}(\mathbf{k})|\neq|\Delta_{ij}(-\mathbf{k})|$). But in the commensurate antiferromagnetic phase, where $\tilde{\varepsilon}_i(\mathbf{k})=\tilde{\varepsilon}_i(-\mathbf{k})$, the coupling $\langle \tilde{a}_i^+(-\mathbf{k})\tilde{a}_i^+(\mathbf{k})\rangle$ is purely triplet and the coupling $\langle \tilde{a}_2^+(-\mathbf{k})\tilde{a}_1^+(\mathbf{k})\rangle$ is purely singlet.

We now turn to the superconducting order parameter $\Delta_{21}(\mathbf{k},\varepsilon_k)$. The substitution of Eqs. (24) and (25) into Eq. (13) yields the following Eliashberg equation[14] (hereafter the subscripts on Δ are omitted):

$$\Delta(\mathbf{k},\varepsilon_k)=[u^2(\mathbf{k})-v^2(\mathbf{k})]\frac{\pi T}{\Omega}\times\sum_{\varepsilon_l}\int\frac{d^2\mathbf{k}'[u^2(\mathbf{k}')-v^2(\mathbf{k}')]}{(2\pi)^3|\nabla\tilde{\varepsilon}_1(\mathbf{k}')|}\times\frac{\Delta(\mathbf{k}',\varepsilon_l)}{[\varepsilon_l^2+\Delta^2(\mathbf{k}',\varepsilon_l)]^{1/2}}g_{\rm ph}^2\frac{\omega_c^2}{\omega_c^2+(\varepsilon_k-\varepsilon_l)^2}. \tag{27}$$

Here we have used the relation $F_{21}^+(\mathbf{k}',\varepsilon_l)=-F_{12}^+(-\mathbf{k}',\varepsilon_l)$. In the commensurate phase, when the factor preceding $\Delta(\mathbf{k}',\varepsilon_l)$ in the integrand of Eq. (27) is invariant under the substitution $\mathbf{k}'\rightarrow-\mathbf{k}'$, only solutions even with respect to $\mathbf{k}'$ and corresponding to singlet coupling are nonzero.

One can easily prove that

$$\Delta(\mathbf{k},\varepsilon_k)=[u^2(\mathbf{k})-v^2(\mathbf{k})]\Delta(\varepsilon_k). \tag{28}$$

Thus, in our model ($g_{\rm ph}$=const), the gap in the spectrum of electron quasiparticles vanishes at the boundaries of breaks in the Fermi surface due to the Bragg planes generated by the magnetic order (if the Bragg planes intersect the Fermi surface). The electron density of states $\nu(\varepsilon)$ in this case is nonzero at all energies ε. At $\varepsilon\ll\Delta_0$, where $\Delta_0=\Delta(\varepsilon_k)$ at $|\varepsilon_k|\ll\omega_c$, the density of states can be estimated to order of magnitude to be

$$\nu(\varepsilon)\sim\varepsilon\nu_0 I_{s-f}S/\Delta_0\varepsilon_F, \tag{29}$$

where ν_0 is the density of electron states at the Fermi surface in the normal phase (see also Ref. 13).

The statement is that the gap is nonzero over the entire Fermi surface at temperatures near T_m if $I_{s-f}<\Delta_0$ derives from an incorrect assumption about the nature of the pairing.

If $g_{\rm ph}\neq$ const, the function $\Delta(\mathbf{k})$ has a more complex form, but nonetheless, near the discontinuities in the Fermi surface, $\Delta(\mathbf{k})$ will be considerably reduced.

We have

$$\Delta(\varepsilon_k)\propto\omega_c\exp(-1/\lambda), \tag{30}$$

where

$$\lambda=g_{\rm ph}^2\int\frac{[u^2(\mathbf{k})-v^2(\mathbf{k})]^2d^2\mathbf{k}}{(2\pi)^3|\nabla\tilde{\varepsilon}_1(\mathbf{k})|}. \tag{31}$$

We first consider the configuration in which the new Bragg planes do not intersect the Fermi surface that exists paramagnetic phase. In this case λ is reduced by $\Delta\lambda$ due to the factor $[u^2(\mathbf{k})-v^2(\mathbf{k})]$:

$$\Delta\lambda/\lambda\sim(I_{s-f}S/Qv_F)^2, \tag{32}$$

where v_F is the Fermi velocity of the electrons. We estimate I_{s-f} from

$$I_{s-f}^2S_{\max}^2\sim T_m\varepsilon_F, \tag{33}$$

where $S_{\max}$ is the saturated holmium spin and T_m is expressed in energy units, yielding

$$\Delta\lambda/\lambda\sim(10^{-3}-10^{-4})\tau,$$

where $\tau=(T_m-T)/T_m$. This negligible change in λ cannot lead to suppression of superconductivity. This is precisely the case in the commensurate phase.

If the new Bragg planes intersect the Fermi surface, which, in our opinion, occurs in the incommensurate phase, each intersection reduces λ by $\Delta\lambda$ such that

$$\Delta\lambda/\lambda\sim I_{s-f}S/Qv_F. \tag{34}$$

Therefore

$$\Delta\lambda/\lambda\sim(10^{-1}-10^{-2})\tau^{1/2}$$

and the suppression of superconductivity is stronger at lower temperatures and higher τ. Hence, it follows that the strong suppression of superconductivity in the incommensurate phase is due to discontinuities in the Fermi surface resulting from magnetic order. This, however, is not sufficient for the total elimination of superconductivity and transition to the normal state. In pure samples with a low concentration of nonmagnetic impurities, superconductivity survives.[6,7] In heavily contaminated materials superconductivity is totally suppressed and a transition to the normal state occurs.[3–5] In our opinion, the differences in behavior among various $HoNi_2B_2C$ samples directly attest to the important role of impurities in suppressing superconductivity.

4. EFFECT OF NONMAGNETIC IMPURITIES ON SUPERCONDUCTIVITY

Suppose that the interaction between electrons and nonmagnetic impurities in the paramagnetic phase is described by the Hamiltonian

$$\mathcal{H}_{e,\rm imp}=\sum_{m,\alpha}\int V_0\delta(\mathbf{r}-\mathbf{R}_m)\psi_{\alpha,\mathbf{k}'}^+(\mathbf{r})\psi_{\alpha,\mathbf{k}}(\mathbf{r})d\mathbf{r}. \tag{35}$$

Here the sum is taken over impurities, $\mathbf{R}_m$ are their coordinates, V_0=const is the potential of the electron–impurity interaction, and $\delta(\mathbf{r})$ is the Dirac delta function. In order to express the Hamiltonian $\mathcal{H}_{e,\rm imp}$ in terms of modified electron wave functions in the antiferromagnetic state, we substitute $\Sigma_m V_0 \exp[i(\mathbf{k}-\mathbf{k}')\mathbf{R}_m]$ for $g_{\text{ph}}[b^+(\mathbf{k}-\mathbf{k}')+b(\mathbf{k}'-\mathbf{k})]$ in Eq. (11).

As in Eq. (27), we obtain the following Eliashberg equation in the presence of impurities:

$$\Delta(\mathbf{k},\varepsilon_k)\left[1+\frac{\pi x}{\Omega}\int\frac{V_0^2 d^2\mathbf{k}'[1+4u(\mathbf{k})u(\mathbf{k}')v(\mathbf{k})v(\mathbf{k}')]}{(2\pi)^3|\nabla\tilde{\varepsilon}_1(\mathbf{k}')|[\varepsilon_k^2+\Delta^2(\mathbf{k}',\varepsilon_k)]^{1/2}}\right]$$

$$=[u^2(\mathbf{k})-v^2(\mathbf{k})]$$

$$\times\left\{\frac{\pi x}{\Omega}\int\frac{d^2\mathbf{k}'[u^2(\mathbf{k}')-v^2(\mathbf{k}')]V_0^2\Delta(\mathbf{k}',\varepsilon_k)}{(2\pi)^3|\nabla\tilde{\varepsilon}_1(\mathbf{k}')|[\varepsilon_k^2+\Delta^2(\mathbf{k}',\varepsilon_k)]^{1/2}}\right.$$

$$+\frac{\pi T}{\Omega}\sum_{\varepsilon_l}\int\frac{d^2\mathbf{k}'[u^2(\mathbf{k}')-v^2(\mathbf{k}')]\Delta(\mathbf{k}',\varepsilon_l)}{(2\pi)^3|\nabla\tilde{\varepsilon}_1(\mathbf{k}')|[\varepsilon_l^2+\Delta^2(\mathbf{k}',\varepsilon_l)]^{1/2}}$$

$$\left.\times g_{\text{ph}}^2\frac{\omega_c^2}{\omega_c^2+(\varepsilon_k-\varepsilon_l)^2}\right\}. \tag{36}$$

In antiferromagnetic superconductors, Anderson's theorem does not hold, and nonmagnetic impurities suppress superconductivity in the same way as paramagnetic impurities in conventional superconductors.[11,12]

Before estimating the critical impurity concentration x_{cr} at which superconductivity is destroyed, we make several remarks.

The typical reciprocal time of electron–impurity scattering, $\tau_0^{-1}\sim xV_0^2\nu_0$, is much larger than $I_{s-f}S$ near T_m. Buzdin and Bulaevskii[13] therefore concluded that in this case electron motion is entirely diffusive, and is not affected by the anisotropy of the magnetic structure, while the gapless band at the Fermi surface disappears.

Because of damping due to impurity scattering, the main contribution to the integral over ξ_i in Eq. (13) is produced by the regions where $\xi_i\sim\tau_0^{-1}$. Therefore the integrands in Eq. (36) are averaged over a range of ξ of order τ_0^{-1}. But this averaging does not affect the factor $u^2(\mathbf{k})-v^2(\mathbf{k})$ preceding the integrals on the right-hand side of Eq. (36) and does not lead to a finite gap at the boundary of the new magnetic Bragg planes, i.e., to the disappearance of the gapless band.

The values of $u^2(\mathbf{k}')-v^2(\mathbf{k}')$ averaged over ξ are essentially the same as the nonaveraged values, since near the new Bragg plane, $\nabla\tilde{\varepsilon}(\mathbf{k}')$ is parallel to this plane, and $u(\mathbf{k}')=v(\mathbf{k}')$ at the intersection. Therefore the decoupling action of impurities does not saturate as their concentration rises. It is described by the parameter τ_s^{-1}, which is similar to the corresponding parameter in the case of paramagnetic impurities in traditional superconductors.[16]

In the commensurate phase, where the magnetic Bragg planes do not intersect the Fermi surface, $|v(\mathbf{k})|\ll 1$, and if the condition $\omega_c\tau_0\ll 1$ is satisfied, $\Delta(\mathbf{k},\varepsilon_k)$ can be considered independent of $\mathbf{k}$.[12,17] In this case Eq. (36) takes the form

$$\Delta(\varepsilon_k)\left\{1+\frac{x}{\Omega}\right.$$

$$\times\int\frac{V_0^2 d^2\mathbf{k}d^2\mathbf{k}'[v(\mathbf{k})+v(\mathbf{k}')]^2}{(2\pi)^2|\nabla\tilde{\varepsilon}_1(\mathbf{k})||\nabla\tilde{\varepsilon}_1(\mathbf{k}')|[\varepsilon_k^2+\Delta^2(\varepsilon_k)]^{1/2}}$$

$$\left.\times\left[\int\frac{d^2\mathbf{k}}{|\nabla\tilde{\varepsilon}_1(\mathbf{k})|}\right]^{-1}\right\}=\frac{\pi T}{\Omega}$$

$$\times\sum_{\varepsilon_l}\int\frac{d^2\mathbf{k}'\Delta(\varepsilon_l)}{(2\pi)^3|\nabla\tilde{\varepsilon}_1(\mathbf{k}')|[\varepsilon_l^2+\Delta^2(\varepsilon_l)]^{1/2}}$$

$$\times g_{\text{ph}}^2\frac{\omega_c^2}{\omega_c^2+(\varepsilon_k-\varepsilon_l)^2}, \tag{37}$$

similar to the equation for the order parameter in a superconductor with paramagnetic impurities[16] and τ_s given by[12]

$$\tau_s^{-1}=\frac{x}{\Omega}\int\frac{V_0^2 d^2\mathbf{k}d^2\mathbf{k}'[v(\mathbf{k})+v(\mathbf{k}')]^2}{(2\pi)^2|\nabla\tilde{\varepsilon}_1(\mathbf{k})||\nabla\tilde{\varepsilon}_1(\mathbf{k}')|}\left[\int\frac{d^2\mathbf{k}}{|\nabla\tilde{\varepsilon}_1(\mathbf{k})|}\right]^{-1}$$

$$\sim\frac{zx(I_{s-f}S)^2}{\varepsilon_F}\sim zT_m\left(\frac{S}{S_{\max}}\right)^2, \tag{38}$$

where z is the number of new Bragg planes. Therefore, as in a superconductor with paramagnetic impurities, gapless superconductivity emerges at $\tau_s^{-1}>\exp(-\pi/4)\Delta_0$, and at $\tau_s^{-1}>0.5\Delta_0$ it is completely destroyed (here Δ_0 is the gap with no impurities).[16] But this must occur at the impurity concentration

$$x_{\text{cr}}\sim\frac{\Delta_0}{T_m z\tau}, \tag{39}$$

hence $x_{\text{cr}}\gtrsim 1$ at $\tau\sim 0.1$. Thus, at realistic impurity concentrations of 10^{-3}–10^{-2} superconductivity is negligibly suppressed by nonmagnetic impurities in the commensurate phase.

In the incommensurate phase, where magnetic Bragg planes intersect the Fermi surface, the major contribution to τ_s^{-1} is due to the regions close to discontinuities of the Fermi surface, where $v(\mathbf{k})\sim 1$. In this case Eq. (36) does not have a simple solution. The result is similar to the case of the commensurate phase, but the characteristic value of τ_s^{-1} is much greater:

$$\tau_s^{-1}\sim xzI_{s-f}S, \tag{40}$$

and

$$x_{\text{cr}}\sim\frac{\Delta_0}{I_{s-f}S_{\max}z\tau^{1/2}}. \tag{41}$$

At $\tau\sim 0.1$ we have $x_{\text{cr}}\sim 10^{-2}$.

Since the decoupling effect of impurities increases with decreasing temperature, i.e., increasing τ, like the effect leading to lower λ owing to the modification of the wave functions, the superconducting state is destroyed at $T_{c2}<T_m$.

5. CONCLUSIONS

1. Superconducting pairing in the helicoidal phase has the form $\langle \tilde{a}_2^+(-\mathbf{k})\tilde{a}_1^+(\mathbf{k})\rangle$.

2. The experimentally observed suppression of superconductivity in the incommensurate phase of $HoNi_2B_2C$ can be consistently accounted for in terms of intersections between new Bragg planes arising due to magnetic order and the paramagnetic-phase Fermi surface.

In the commensurate phase the magnetic Bragg planes are far from the Fermi surface because of the difference between the wave vectors of magnetic order in the commensurate and helicoidal phases, so the effect of magnetic order on superconductivity in the commensurate phase is considerably weaker.

3. The superconductivity is gapless, i.e., the gap vanishes at the intersections with the new Bragg planes throughout the temperature range where the helicoidal phase occurs, up to T_m.

4. Nonmagnetic impurities suppress superconductivity in the case of long-range antiferromagnetic order. The amplitude of the effect of magnetic order on superconductivity is different in different $HoNi_2B_2C$ samples because of vanishing impurity concentrations.

5. There is no temperature range in which the decoupling action of impurities is saturated and independent of the impurity concentration.

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