Nonphonon superconductivity of planar nickel borides

R. O. Zaĭtsev

Kurchatov Institute, 123182 Moscow, Russia

Yu. V. Mikhaĭlova

State Research Institute of Thermal-Power Instrument Engineering, 129085 Moscow, Russia

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The electronic structure of the conduction band is studied in the limit of infinitely high positive Hubbard energy. The partial scattering amplitudes are calculated, the conditions for Cooper instability are determined on their basis, and a diagram for the existence of a superconducting state is constructed. © *1996 American Institute of Physics.* [S1063-7761(96)02405-5]

1. INTRODUCTION

The suggestion[1] that there is a strong electron–phonon interaction (with a BCS constant $\lambda=2.6$) in the compound $Lu(NiB)_2C$ is at variance with the quadratic temperature dependence of the resistivity observed in Ref. 2. The alternative suggestion of a weak electron–electron interaction U contradicts the estimates in Ref. 3, according to which the value of U for nickel $3d$ compounds is 20 eV. This exceeds the value of the transfer integral between nickel and boron, $t\cong 2$ eV, whence it can be concluded that U is the largest energy parameter, which will be considered infinite below. Similar arguments are applicable to the boron $2p$ states with the same crystal indices, enabling us to single out the lowest two-particle states on the basis of Hund's rule and to neglect transitions to singlet states.

In the $Lu(NiB)_kC$ compounds studied the boron and carbon $2s$ states are filled, while the nickel $4s$ states are unfilled, so that the mean occupation numbers of the boron $2p$ subshell ($\bar{n}_p$) and of the nickel $3d$ subshell ($\bar{n}_d$) are related to one another by the chargeneutrality equation

$$\bar{n}_p+\bar{n}_d=11+Q/k \quad \text{or} \quad n_p+n_d=5-Q/k, \tag{1}$$

where $n_p=6-\bar{n}_p$, $n_d=10-\bar{n}_d$ is the mean number of holes in the boron and nickel $2p^6$ and $3d^{10}$ subshells, and Q is the total charge of the complex LuC: $Q=Q_{Lu}+Q_C$. According to the calculations in Ref. 1, the carbon $2p$ subshell contains no more than two electrons, i.e., $0<Q_C\leqslant +2$. When the Lu $4f$ subshell is filled, the maximum number of Lu $5d$ electrons does not exceed four, i.e., $3\geqslant Q_{Lu}>-1$. Therefore, $-1<Q\leqslant 5$, and our task is to consider the filling range $0<n_d<4$ with simultaneous filling of the $p_{x,y}$ hole levels in the range $4>n_p>0$. The ranges $4<n_d<9/2$, $1/2>n_p>0$, $4<n_p<9/2$, and $1/2>n_d>0$ are not considered, since superconductivity does not exist within them due to the small number of both p and d excitations.[4]

Nickel cations form a square planar lattice with the second cation located at the center of the square at a distance of 2.45 Å from the first. Two boron layers, which also form a square lattice are at small distances above and below the nickel lattice, so that the closest distance between nickel and boron atoms (2.11 Å) is smaller than the distance between nickel cations and the distance between boron anions (3.46 Å), which is equal to the lattice constant.

2. EQUATIONS OF STATE

Thus, in writing the Hamiltonian it is sufficient to take into account only the transitions between neighboring Ni and B planar sublattices:

$$\hat{H}=\sum_{\mathbf{r},\mathbf{r}'}{}' [t^{\lambda,\nu}_{\mathbf{r},\mathbf{r}'}\hat{d}^+_{\mathbf{r}\sigma}(\lambda)\hat{p}_{\mathbf{r}'\sigma}(\nu)+\text{h.c.}]$$

$$+\sum_{\mathbf{r}\sigma\lambda}\varepsilon_d\hat{d}^+_{\mathbf{r}\sigma}(\lambda)\hat{d}_{\mathbf{r}\sigma}(\lambda)+\sum_{\mathbf{r}\sigma\nu}\varepsilon_p\hat{p}^+_{\mathbf{r}\sigma}(\nu)\hat{p}_{\mathbf{r}\sigma}(\nu). \tag{2}$$

Here $\hat{d}^+_{\mathbf{r}\sigma}(\lambda)$, $\hat{p}^+_{\mathbf{r}\sigma}(\nu)$, $\hat{d}_{\mathbf{r}\sigma}(\lambda)$, and $\hat{p}_{\mathbf{r}\sigma}(\nu)$ are the creation and annihilation operators of holes in the nickel or boron d and p subshells. The indices λ and ν label the layers, as well as the atomic states, which are degenerate. The energies ε_p and ε_d do not depend on the spin index σ, on the crystal index of the $p_{x,y}$ states, or on the number of the sublattice.

Note that the matrix elements of the p_x states are nonzero only for transitions in the xz plane, since the boron p_x states are orthogonal to the (x^2-y^2) or $(3z^2-r^2)$ states of the nickel cations, which are displaced relative to boron in the yz plane.

We first consider the filling of the lowest (x^2-y^2) level. Here the transition matrix between the nickel a and b sublattices and the upper and lower boron layers is proportional to the following matrix:

$$\hat{M}=\begin{pmatrix} 0 & \nu_x & -\nu_y & 0 \\ \nu_x^* & 0 & 0 & -\nu_y^* \end{pmatrix}. \tag{3}$$

Here $\nu_k=1-\exp(iq_k)$. The first and second rows correspond to atoms in the nickel a and b sublattices, and the first and third (second and fourth) columns correspond to x and y states belonging to the upper (lower) boron layer.

For the filling of the Ni $(3z^2-r^2)$ level, we have the same matrix, but with the opposite sign in the last two columns.

When transitions between the states $|0\rangle$ with a filled shell and the states $\hat{d}_\sigma^+|0\rangle$ or $\hat{p}_{k\sigma}^+|0\rangle$ with one hole are considered, the creation and annihilation operators are equal to the corresponding X operator:

$$\hat{d}_{\mathbf{r}\sigma}^+=\hat{X}_{\mathbf{r}}^{(\sigma,0)}, \quad \hat{d}_{\mathbf{r}\sigma}=\hat{X}_{\mathbf{r}}^{(0,\sigma)}, \quad \hat{p}_{\mathbf{r}\sigma}^+(k)=\hat{Y}_{\mathbf{r}}^{(k\sigma,0)},$$

$$\hat{p}_{\mathbf{r}\sigma}(k)=\hat{Y}_{\mathbf{r}}^{(0,k\sigma)}. \tag{4}$$

Transitions between unoccupied and one-particle (x^2-y^2) states in terms of holes are transitions between two-hole $(\hat{d}_\sigma^+\hat{d}_{\bar{\sigma}}^+|0\rangle)$ and one-hole states (here and in the following $\bar{\sigma}=-\sigma=\pm 1$):

$$\hat{d}_{\mathbf{r}\sigma}^+=\sigma\hat{X}_{\mathbf{r}}^{(2,\bar{\sigma})}, \quad \hat{d}_{\mathbf{r}\sigma}=\sigma\hat{X}_{\mathbf{r}}^{(\bar{\sigma},2)}, \tag{5}$$

When the $(3z^2-r^2)$ level is filled, we have the same relations, but with the replacement of $\hat{X}$ by $\hat{Z}$.

In the case of $1<n_p<2$, transitions between the four one-hole states in the $p_{x,y}$ subshell $\hat{p}_{k\sigma}^+|0\rangle$ $(k=x,y;\ \sigma=\pm)$ and the three two-hole states $\hat{p}_{x\sigma}^+\hat{p}_{y\sigma}^+|0\rangle$ $(S=1,\ S_z=\sigma=\pm 1)$ and $(\hat{p}_{x\sigma}^+\hat{p}_{y\bar{\sigma}}^++\hat{p}_{x\bar{\sigma}}^+\hat{p}_{y\sigma}^+)/\sqrt{2}|0\rangle$ $(S=1,\ S_z=0)$. As a result we have

$$\hat{p}_{\mathbf{r}x\sigma}^+=\hat{Y}_{\mathbf{r}}^{1,\sigma;y,\sigma}+\frac{1}{\sqrt{2}}\hat{Y}_{\mathbf{r}}^{1,0;y,\bar{\sigma}}, \quad \hat{p}_{\mathbf{r}y\sigma}^+=-\hat{Y}_{\mathbf{r}}^{1,\sigma;x,\sigma}$$

$$-\frac{1}{\sqrt{2}}\hat{Y}_{\mathbf{r}}^{1,0;x,\bar{\sigma}}, \tag{6}$$

$$\hat{p}_{\mathbf{r}x\sigma}=\hat{Y}_{\mathbf{r}}^{y,\sigma;1,\sigma}+\frac{1}{\sqrt{2}}\hat{Y}_{\mathbf{r}}^{y,\bar{\sigma};1,0}, \quad \hat{p}_{\mathbf{r}y\sigma}=-\hat{Y}_{\mathbf{r}}^{x,\sigma;1,\sigma}$$

$$-\frac{1}{\sqrt{2}}\hat{Y}_{\mathbf{r}}^{x,\bar{\sigma};1,0}.$$

There is no need to write out the relations referring to the range $2<n_p<4$, since the final results are invariant with respect to the particle–hole symmetry transformation $n_d\to 2-n_d$, $n_p\to 4-n_p$.

A comparison of the expansions (4) and (6) reveals that in the range $1<n_p<2$ all the one-particle p operators acquire a second index, which corresponds to transitions to a state with zero spin projection $|S=1,0\rangle$.

The one-particle Green's function is defined by the following matrix inverse:

$$\hat{G}^{-1}=\begin{pmatrix} \hat{\Omega}_d & -f_d t\hat{M} \\ -f_p b_k^{(\alpha)} t\hat{M}^+ & \hat{\Omega}_p \end{pmatrix}, \tag{7}$$

where $\hat{\Omega}_d=(i\omega-\varepsilon_d)\hat{I}$ is a two-component unit matrix belonging to two identical Ni cations, and $\hat{\Omega}_p=(i\omega-\varepsilon_p)\hat{I}$ is a four-component matrix belonging to a layer of boron atoms, each of which is found in a p_x or p_y state, above or below the Ni layer. The quantity t is the matrix element for a transition between nearest neighbor nickel and boron atoms. The factors f_p and f_d are the so-called end multipliers,[4] which are linear functions of the mean occupation numbers n_p or n_d in the case of an infinite Hubbard energy. At the boundary of each of the integer ranges, the value of the end multiplier is equal to the reciprocal of the degeneracy of the multiplicity of the lower level. Accordingly,

$$f_d=\begin{cases} 1-n_d/2 & \text{for } 0<n_d<1, \\ n_d/2 & \text{for } 1<n_d<2, \end{cases}$$

$$f_p=\begin{cases} 1-3n_d/4 & \text{for } 0<n_p<1, \\ (2+n_d)/12 & \text{for } 1<n_p<2. \end{cases} \tag{8}$$

We find the multipliers f_p for the range $2<n_p<4$ using the particle–hole symmetry transformation $n_p\to 4-n_p$.

The multipliers $b_k^{(\alpha)}$ are the so-called parentage coefficients, which, according to (4)–(6), can be used to expand the creation and annihilation operations in Hubbard $\hat{X}$ operators:

$$b_k=1 \quad \text{for} \quad 0<n_p<1 \quad \text{and} \quad 3<n_p<4, \tag{9}$$

$$b_x^{(\alpha)}=(1,1/\sqrt{2}), \quad b_y^{(\alpha)}=(-1,-1/\sqrt{2}) \text{ for } 1<n_p<3.$$

After calculating the determinant of the inverse Green's function (7), we find the excitation spectrum, which has fourfold degeneracy (with respect to the spin, as well as replacement of the a and b sublattices):

$$\xi_{\mathbf{p}}^{(\pm)}=\pm\sqrt{(r/2)^2+b_p^2 f_p f_d t^2 J(\mathbf{p})}-\mu, \tag{10}$$

where $r=\varepsilon_p-\varepsilon_d$, $\mu=-(\varepsilon_p+\varepsilon_d)/2$, and the other two branches of the spectrum remain localized at the level of ε_p; $J(\mathbf{p})=2(2-\cos p_x-\cos p_y)$, $b_p^2=1$ for $0<n_p<1$ and $3<n_p<4$; $b_p^2=3/2$ for $1<n_p<3$.

After calculating the diagonal matrix elements of the one-particle Green's function $\hat{G}$ in terms of the inverse matrix (7) and multiplying by the corresponding end multiplier (8), we find the equations of state:

$$n_d=2f_d\sum_{\mathbf{p}\lambda=\pm} a_{\mathbf{p}}^{(-\lambda)} n_F(\xi_{\mathbf{p}}^{(\lambda)}), \quad 0<n_d<1, \tag{11a}$$

$$n_d=1+f_d\sum_{\mathbf{p}\lambda=\pm} a_{\mathbf{p}}^{(-\lambda)} n_F(\xi_{\mathbf{p}}^{(\lambda)}), \quad 1<n_d<2, \tag{11b}$$

$$n_p=2f_p\sum_{\mathbf{p}}\left\{n_F(\varepsilon_p)\right.$$

$$\left.+\sum_{\lambda=\pm} a_{\mathbf{p}}^{(+\lambda)} n_F(\xi_{\mathbf{p}}^{(\lambda)})\right\}, \quad 0<n_p<1, \tag{11c}$$

$$n_p=1+\frac{3}{2}f_p\sum_{\mathbf{p}}\left\{n_F(\varepsilon_p)+\sum_{\lambda=\pm} a_{\mathbf{p}}^{(+\lambda)} n_F(\xi_{\mathbf{p}}^{(\lambda)})\right\},$$

$$1<n_p<2. \tag{11d}$$

The end multipliers and the excitation spectrum are determined from (8) and (10); the normal coordinates $a_{\mathbf{p}}^{(\pm)}$ have the following form:

$$a_{\mathbf{p}}^{(\pm)}=\frac{1}{2}\left\{1\pm\frac{r/2}{\sqrt{(r/2)^2+b_p^2 f_p f_d t^2 J(\mathbf{p})}}\right\}. \tag{12}$$

The remaining equations of state for the range $4>n_p>2$ can be obtained using the particle–hole symmetry transformation

$n_d \to 2-n_d$, $n_p \to 4-n_p$. The equations of state in the case of filling of the $(3z^2-r^2)$ level are obtained from (8) and (11) using the replacement $n_d \to n_d-2$.

3. SUPERCONDUCTIVITY CRITERIA

To find the conditions for Cooper instability,[6] we represent the system of ladder equations for the two-particle vertex part written for zero total momentum and spin in the form

$$\Gamma_{\alpha\bar{\mu};\lambda\bar{\nu}}(\mathbf{p}) = \Gamma^{(0)}_{\alpha\bar{\mu};\lambda\bar{\nu}}(\mathbf{p}) - T\sum_{\omega,\mathbf{p}'} \Gamma^{(0)}_{\alpha\bar{\mu};\alpha'\bar{\mu}'}(\mathbf{p}') \times G^{\alpha'\lambda'}_{\omega}(\mathbf{p}') G^{\bar{\mu}'\bar{\nu}'}_{-\omega}(-\mathbf{p}') \Gamma_{\lambda'\bar{\nu}';\lambda\bar{\nu}}(\mathbf{p}'), \tag{13}$$

where T is the temperature. The vertex part $\Gamma^{(0)}_{\alpha\bar{\mu};\lambda\bar{\nu}}(\mathbf{p}')$ is the sum of the diagrams which are irreducible with respect to cutting along two electron lines in the same direction. The indices without a bar (and with a bar) label transitions with an assigned positive (and negative) sign for the change in spin projection. Restricting ourselves to logarithmic accuracy, we determine the vertex part $\Gamma^{(0)}_{\alpha\bar{\mu};\beta\bar{\nu}}$ in the simplest Born approximation. According to Refs. 5, 7, and 8, the Born amplitude $\Gamma^{(0)}_{\alpha\bar{\mu};\lambda\bar{\nu}}(\mathbf{p})$ is determined in terms of the coefficients of the operators $\hat{X}^{\lambda}$ and $\hat{X}^{\nu'}$ after calculating the double commutation relation $\{\hat{X}^{\alpha},[\hat{X}^{\bar{\mu}},\hat{H}]\}$.

The tunneling Hamiltonian (2) can be represented as a sum of two terms

$$\hat{H} = \sum_{\mathbf{r}\mathbf{r}'}{}' \{\hat{X}^{\nu}_{\mathbf{r}} t^{\nu\mu}(\mathbf{r},\mathbf{r}')\hat{X}^{\mu}_{\mathbf{r}'} + \hat{X}^{\bar{\nu}}_{\mathbf{r}} t^{\bar{\nu}\bar{\mu}}(\mathbf{r},\mathbf{r}')\hat{X}^{\bar{\mu}}_{\mathbf{r}'}\}, \tag{14}$$

after which the commutator can be expressed in terms of the tunneling transition matrix $t^{\alpha\beta}(\mathbf{r},\mathbf{r}') = b^{\alpha}_i t^{ik}(\mathbf{r}-\mathbf{r}')b^{\beta}_k$ and the structure constants $N^{(\pm)}_{\alpha,\beta}$ of the corresponding superalgebra:

$$[X^{\alpha}_{\mathbf{r}}, X^{\beta}_{\mathbf{r}'}]_{\pm} = N^{(\pm)}_{\alpha,\beta} X^{\alpha+\beta}_{\mathbf{r}} \delta_{\mathbf{r},\mathbf{r}'},$$

$$[X^{\alpha}_{\mathbf{r}}, \hat{H}] = \sum_{\mathbf{r}'\nu} (N^{(+)}_{\alpha,\nu} X^{\alpha+\nu}_{\mathbf{r}} t^{\nu;\beta}(\mathbf{r},\mathbf{r}') X^{\beta}_{\mathbf{r}'} + (\nu \to \bar{\nu}; \beta \to \bar{\beta})).$$

Finally, after calculating the anticommutator $\{X^{\mu}_{\mathbf{r}},[X^{\bar{\mu}}_{\mathbf{r}},\hat{H}]\}$ and going to the Fourier representation, we find

$$\Gamma^{(0)}_{\mu\bar{\mu};\nu\bar{\nu}}(\mathbf{p}_3 = -\mathbf{p}_4 = \mathbf{p}) = N^{(+)}_{\mu,\bar{\nu}-\mu-\bar{\mu}} N^{(-)}_{\bar{\mu},\bar{\nu}-\bar{\mu}} t^{\bar{\nu}-\bar{\mu}-\mu,\nu}(\mathbf{p}) + N^{(+)}_{\bar{\mu},\nu-\bar{\mu}-\mu} N^{(-)}_{\mu,\nu-\mu} t^{\nu-\mu-\bar{\mu},\bar{\nu}}(-\mathbf{p}). \tag{15}$$

Substituting this expression instead of Γ_0 into (13), we find that the left-hand side of the corresponding homogeneous system of equations does not depend on the relative momentum $\mathbf{p}$. After the substitution of (15) into the homogeneous system of equations corresponding to (13), we carry out the summation over the internal indices ν and $\bar{\nu}$ using the Dyson equation, which has been used already to find the inverse Green's function (7):

$$[(\hat{G}^{(0)}_{\omega})^{-1}\hat{G}_{\omega}(\mathbf{p})]^{\alpha}_{\beta} = \delta_{\alpha,\beta} - f_{\alpha} t^{-\alpha,\nu}(\mathbf{p}) G^{\nu,\beta}_{\omega}(\mathbf{p}), \tag{16}$$

$$[(\hat{G}^{(0)}_{\omega})^{-1}\hat{G}_{-\omega}(-\mathbf{p})]^{\alpha}_{\beta} = \delta_{\alpha,\beta} - f_{\alpha} t^{-\alpha,\bar{\nu}}(\mathbf{p}) G^{\bar{\nu},\beta}_{-\omega}(-\mathbf{p}).$$

Multiplying the first relation by $G^{-\omega}(-\mathbf{p})$ and the second relation by $G_{\omega}(\mathbf{p})$ and neglecting the nonlogarithmic terms containing the first powers of the Green's functions, we obtain the following homogeneous system

$$\Gamma_{\alpha,\bar{\alpha}} = -T\sum_{\omega,\mathbf{p}} g_{\alpha\bar{\alpha};\mu\bar{\mu}'} G^{\mu\lambda'}_{\omega}(\mathbf{p}) G^{\bar{\mu}'\bar{\nu}'}_{-\omega}(-\mathbf{p}) \Gamma_{\lambda'\bar{\nu}'}. \tag{17}$$

Here the coefficients $g_{\alpha\bar{\alpha};\mu\bar{\mu}}$ no longer depend on the momentum and are defined in terms of $\Gamma^{(0)}(\mathbf{p})$ in (15):

$$g_{\mu\bar{\mu};\nu\bar{\nu}} = N^{(+)}_{\mu,\bar{\nu}-\bar{\mu}-\mu} N^{(-)}_{\bar{\mu},\bar{\nu}-\bar{\mu}} f^{-1}_{\mu+\bar{\mu}-\bar{\nu}} [(\hat{G}^{(0)}_{\omega})^{-1}]^{\mu+\bar{\mu}-\bar{\nu}}_{\nu} + N^{(+)}_{\bar{\mu},\nu-\mu-\bar{\mu}} N^{(-)}_{\mu,\nu-\mu} f^{-1}_{\bar{\mu}+\mu-\nu} [(\hat{G}^{(0)}_{\omega})^{-1}]^{\mu+\bar{\mu}-\nu}_{\bar{\nu}}. \tag{18}$$

The inverse zeroth Green's function $\{\hat{G}^{(0)}_{\omega}\}^{-1}$ has only diagonal matrix elements, so that the end multipliers $f_{\mu+\bar{\mu}-\bar{\nu}}$ and $f_{\bar{\mu}+\mu-\nu}$ are sums of the occupation numbers of the initial and final states for the ν and $\bar{\nu}$ transitions.

Note that the matrix elements of the one-particle Green's functions $G_{\omega}(\mathbf{p})$ for a given value of the crystal index k depend on the number of the transition only through the product of the parentage coefficients b^{α}_k

$$G^{\mu\nu}_{\omega}(\mathbf{p}) = b^{\mu}_k b^{\nu}_s G^{ks}_{\omega}(\mathbf{p}). \tag{19}$$

Substituting (19) into (17), we obtain the equations for the functions $\Gamma_{ks} = b^{\mu}_k b^{\bar{\nu}}_s \Gamma_{\mu\bar{\nu}}$, which do not depend on the number of the transition:

$$\Gamma_{k\bar{s}} = -T\sum_{\omega,\mathbf{p}} \tilde{g}_{k\bar{s};n\bar{m}} G^{nn'}_{\omega}(\mathbf{p}) G^{\bar{m}\bar{m}'}_{-\omega}(-\mathbf{p}) \Gamma_{n'\bar{m}'}, \tag{20}$$

where we now have

$$\tilde{g}_{k\bar{s};n\bar{m}} = b^{\mu}_k b^{\bar{\mu}}_{\bar{s}} g_{\mu\bar{\mu};\nu\bar{\nu}} b^{\nu}_n b^{\bar{\nu}}_{\bar{m}}. \tag{21}$$

In the range $0<n_p<1$ all the parentage coefficients are equal to unity, and the problem reduces to solving a system of equations for two parameters, viz., $\Gamma_{xx} = \Gamma_{yy} = \Gamma_p$ and Γ_d. In this case $\tilde{g}_{xx;xx} = \tilde{g}_{yy;yy} = -2\Omega_p/f_p$. According to (9), for the range $1<n_p<2$ we have four coefficients for the transitions to states with the maximum spin projection $b^{(2)}_{x,y} = \pm 1$, while for the transitions to a state with a zero spin projection $b^{(3)}_{x,y} = \pm 1/\sqrt{2}$. For a given index $g_{2\bar{2};2\bar{2}} = g_{3\bar{2};2\bar{3}} = g_{2\bar{3};3\bar{2}} = 0$, and $g_{2\bar{3};2\bar{3}} = g_{3\bar{2};3\bar{2}} = -g_{3\bar{3};3\bar{3}} = -2\Omega_p/f_p$, so that after summation according to Eq. (21), we obtain $g_{xx;xx} = g_{yy;yy} = -3\Omega_p/2f_p$. The analogous calculations for the scattering amplitude of the d excitations give $\tilde{g}_{dd;dd} = \mp 2\Delta_d/f_d$, where the upper sign $(-)$ is taken for occupation numbers in the range $0<n_d<1$, and the lower sign $(+)$ is taken for occupation numbers in the range $1<n_d<2$.

The off-diagonal components of the Green's functions $G^{sn}_{\omega}(\mathbf{p})$ on the right-hand side of Eq. (20) are determined using (19):

$$G^{xy}_{\omega}(\mathbf{p}) = \frac{f_p \nu_x \nu^*_y f_d}{\Delta\Omega_p}, \quad G^{yx}_{\omega}(\mathbf{p}) = \frac{f_p \nu_y \nu^*_x f_d}{\Delta\Omega_p},$$

$$G^{kd}_{\omega}(\mathbf{p}) = \frac{f_p \nu_k}{\Delta}, \quad G^{dk}_{\omega}(\mathbf{p}) = \frac{f_p \nu^*_k}{\Delta},$$

$$k=x,y, \quad \Delta=\Omega_p\Omega_d-b_p^2f_pf_dJ(\mathbf{p}).$$

For the diagonal components $G_\omega^{kk}(\mathbf{p})$ the representation (19) is valid when $\Delta\to 0$ and $\Omega\neq 0$, i.e., when the $\xi_{\mathbf{p}}^{(\pm)}$ subbands are filled, but $\varepsilon_p\neq 0$:

$$G_\omega^{xx}(\mathbf{p})\cong\frac{f_pf_d|\nu_x|^2}{\Delta\Omega_p}, \quad G_\omega^{yy}(\mathbf{p})\cong\frac{f_pf_d|\nu_y|^2}{\Delta\Omega_p},$$

$$G_\omega^{dd}(\mathbf{p})\cong\frac{\Omega_p}{\Delta}. \tag{22}$$

Substitution of these functions and integration of the expressions obtained near one of the Fermi surfaces give the following system:

$$\Gamma_p=-g_p\left\{\frac{1}{2}f_p^2f_d^2\overline{[|\nu_x|^2+|\nu_y|^2]^2}\Gamma_p+\frac{1}{2}f_p^2\overline{\Omega_p^2[|\nu_x|^2+|\nu_y|^2]}\Gamma_d\right\}, \tag{23}$$

$$\Gamma_d=-g_d\{f_d^2\overline{[|\nu_x|^2+|\nu_y|^2]}\Omega_p^2\Gamma_p+\overline{\Omega_p^4}\Gamma_d\}.$$

The overbar denotes multiplication by $T^2|\Delta_\omega\Delta_p|^{-2}$ and further summation over all momenta and frequencies ω. Taking into account that the integration over the momenta is carried out in the region where $\Delta\to 0$ and $\varepsilon_p\neq 0$, we must replace the expression $J(\mathbf{p})=[|\nu_x|^2+|\nu_y|^2]$ by $\Omega_p\Omega_d/b_p^2f_pf_d$, and we must replace Ω_p and Ω_d by $-\varepsilon_p$ and $-\varepsilon_d$, respectively. As a result, we obtain

$$g_d=2\frac{\varepsilon_d\gamma_d}{f_d}, \quad \text{where} \quad \gamma_d=\begin{cases}1 & \text{for} \quad 0<n_d<1,\\ -1 & \text{for} \quad 1<n_d<2;\end{cases} \tag{24a}$$

$$g_p=2\frac{\varepsilon_p\gamma_p}{f_d}, \quad \text{where} \quad \gamma_p=\begin{cases}1 & \text{for} \quad 0<n_p<1,\\ 3/4 & \text{for} \quad 1<n_p<2.\end{cases} \tag{24b}$$

As a result of some simple transformations, we obtain the following solvability condition:

$$-\varepsilon_p\varepsilon_d\left\{\gamma_p\frac{\varepsilon_d}{2b_p^4f_p}+\gamma_d\frac{\varepsilon_p}{f_d}\right\}\times T\sum_{\omega,\mathbf{p}}\frac{2}{[\omega^2+(\xi_{\mathbf{p}}^{(+)})^2][\omega^2+(\xi_{\mathbf{p}}^{(-)})^2]}=1. \tag{25}$$

Using the density of states $\rho_\pm=\Sigma\delta(\xi_{\mathbf{p}}^{(\pm)})$, we can transform the condition (25) into a relation of the BCS form $T_c\approx t^*\exp(-1/\lambda_\pm)$, where

$$\lambda_\pm=-\rho_\pm\frac{\varepsilon_p\varepsilon_d}{2\mu^2}\left\{\gamma_p\frac{\varepsilon_d}{2b_p^4f_p}+\gamma_d\frac{\varepsilon_p}{f_d}\right\}. \tag{26}$$

The value of t^* is of the order of the transfer integral t, but it cannot be calculated within the logarithmic approximation used. It can easily be shown that the product $\varepsilon_p\varepsilon_d$ has a positive sign when the $\xi_{\mathbf{p}}^{(+)}$ or $\xi_{\mathbf{p}}^{(-)}$ subband is filled, so that the condition for the existence of superconductivity is as follows:

TABLE I.

Range	γ_p	γ_d	f_p	f_d	b_p^2
$0<n_d<1, 0<n_p<1$	1	1	$1-3n_p/4$	$1-n_d/2$	1
$0<n_d<1, 1<n_p<2$	3/4	1	$(2+n_p)/12$	$1-n_d/2$	3/2
$1<n_d<2, 0<n_p<1$	1	−1	$1-3n_p/4$	$n_d/2$	1
$1<n_d<2, 1<n_p<2$	3/4	1	$(2+n_p)/12$	$n_d/2$	3/2

$$\gamma_p\frac{\varepsilon_d}{2b_p^4f_p}+\gamma_d\frac{\varepsilon_p}{f_d}\leqslant 0. \tag{27}$$

The equality sign corresponds to the boundary for the appearance of the superconducting state. Combining (27) with the equations of state, we find the region where the superconducting phase exists in the variables n_p and n_d (see Fig. 1).

The parameters in the basic relations (26) and (27) are listed in Table I.

4. PHASE DIAGRAM

In the first two cases, in which both scattering amplitudes γ_p and γ_d are positive, the condition for the appearance of superconductivity must be satisfied for negative ε_p and ε_d, i.e., when the upper $\xi_{\mathbf{p}}^{(+)}$ subband is filled. Using the equations of state (11), we find two regions:

1) $4(4-3n_d)/(16-11n_d)<n_p<1, \quad 0<n_d<1,$ (28a)

2) $2(12-7n_d)/(12-5n_d)<n_p<2, \quad 0<n_d<1.$ (28b)

For the upper Hubbard band of $e_{\mathbf{p}}$ holes, where $1<n_d<2$, when the lower $\xi_{\mathbf{p}}^{(-)}$ subband is filled, superconductivity exists owing to the pairing of d electrons. For the range $4/3<n_d<2$ and $r>0$ superconductivity appears at any degree of filling of the $\xi^{(-)}$ subband. According to the equations of state, this condition corresponds to the following regions:

$$0<n_p<4(2-n_d)/(6-n_d), \quad 4/3<n_d<2, \tag{29a}$$

$$1<n_p<2(2+3n_d)/(9n_d-2), \quad 4/3<n_d<2. \tag{30a}$$

These two regions are adjoined on the sides of the range $1<n_d<4/3$ by two more regions corresponding to $r<0$, whose boundary is defined when the density of the p excitations is finite. They have a positive scattering amplitude, which results in a decrease in the effective constant λ and further disappearance of the Cooper instability as the density of the p states increases. The superconducting regions are defined implicitly by the condition that the corresponding BCS constants vanish. Combining these conditions with the equation of state, we find the regions for the existence of superconductivity for $0<n_d<4/3$

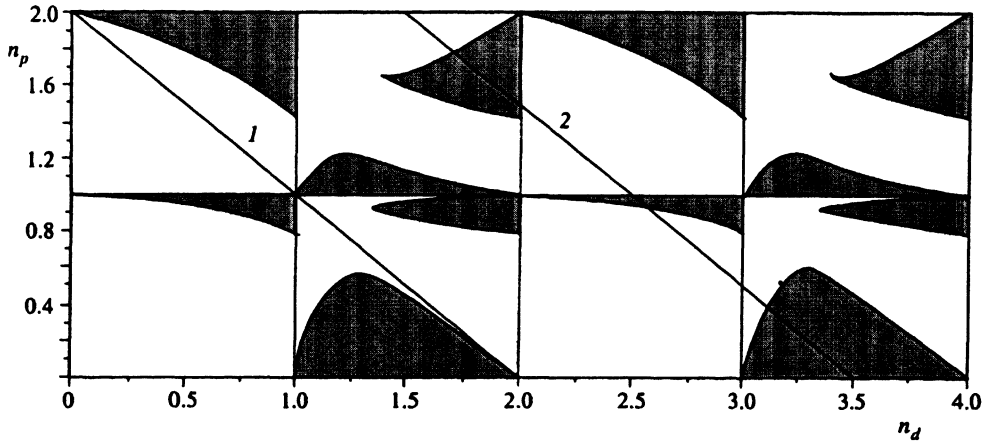

FIG. 1. Phase diagram for the existence of a superconducting state at $T=0$. The superconducting regions are shaded; *1*—chargeneutrality line for LuNiBC; *2*—chargeneutrality line for $Lu(NiB)_2C$. The calculations were performed in the flat-band model.

$$0<n_p<\Phi_1(n_d), \tag{29b}$$

$$1<n_p<\Phi_2(n_d). \tag{30b}$$

According to numerical calculations in the flat-band model, the function $\Phi_1(n_d)$ has maximum value 0.56 when $n_d=1.26$. The function Φ_2 also has maximum value 1.23 when $n_d=1.23$.

When the upper $\xi_{\mathbf{p}}^{(+)}$ subband is filled, superconductivity results mainly from the appearance of a negative $p-p$ scattering amplitude. For $4/5<n_p<1$ and $\varepsilon_p<\varepsilon_d<0$ superconductivity appears from the very onset of the filling of the $\xi_{\mathbf{p}}^{(+)}$ subband:

$$(4-3n_p)/n_p<n_d<2, \quad 4/5<n_p<12/13, \tag{31a}$$

$$\Phi_3(n_p)<n_d<2, \quad 12/13<n_p<1. \tag{31b}$$

Here the region (31b) corresponds to filling of the $\xi_{\mathbf{p}}^{(+)}$ subband when $0>\varepsilon_p>\varepsilon_d$, and Φ_3 is specified by the condition $g=0$, which corresponds to an increase in the role of $d-d$ scattering with a positive scattering amplitude as the number of $(2-n_d)$-electron d excitations increases.

Superconductivity originating from p excitations also exists in the range $10/7<n_p<2$. This region is defined in the variables n_d and n_p by the following equalities:

$$2(1+2n_d)/(4n_d-1)<n_p<\Phi_4(n_d) \text{ for } 4/3<n_d<2. \tag{32}$$

The function Φ_4 is specified by the condition $g=0$ and by the equations of state for $\varepsilon_p<\varepsilon_d<0$. When $n_d=4/3$, for which $n_p=22/13\cong 1.69$, Φ_4 is also equal to 22/13. The function Φ_4 decreases in the range $4/3<n_d<1.43$, and when $n_d=1.43$, it has its minimum value, which equals 1.66, and then increases to a value of 2.

The remainder of the phase diagram for $2<n_p<4$ can be obtained from the region $n_p<2$ using the particle–hole symmetry transition formation $n_p\to 4-n_p$, $n_d\to 2-n_d$ (see Fig. 1). The second half of the phase diagram $2<n_d<4$, where filling of the $(3z^2-r^2)$ subband occurs, is found using the shift operation $n_d\to n_d-2$.

As follows from Fig. 1, in the region $n_p<1$, $0<n_d<2$ the phase diagram does not differ qualitatively from the phase diagrams of compounds containing CuO_2 layers.[9] However, superconductivity cannot exist for the analogous compounds with NiO_2 layers due to the small number of excitations at the small values $2-n_d$ and $n_p\ll 1$, i.e. in the region where the chargeneutrality line passes for $Ln_{2-x}M_x^{2+}NiO_4$.

In the case of a filled carbon $2p_z$ level (C^0) and an empty lutetium $5d$ subshell (Lu^{3+}), we have $n_p+n_d=7/2$ for the chargeneutrality line.

Thus, when the nickel $3z^2-r^2$ level is filled, superconductivity exists mainly due to hole pairing of d electron excitations. The p hole excitations have a positive scattering amplitude, which leads to restriction of the region where the superconducting state exists when $n_p>0.4$ (see Fig. 1). Another possibility appears in the region $2<n_d<3$, $n_p>4/5$, which is also intersected by the chargeneutrality line. Here the possibility of superconductivity is also due to negative $d-d$ and $p-p$ scattering amplitudes.

When the (x^2-y^2) level is filled and, according to the chargeneutrality condition, $3/2<n_p<2$, the electronic $p_{x,y}$ subshell is almost half filled, superconductivity appears mainly because of a negative $p-p$ scattering amplitude. Thus, the suggestion that the carbon p_x level is completely filled and the shell of the Lu^{3+} cations is maximally stable makes it possible to account for nonphonon superconductivity of the same type as in CuO_2 layers.

As is seen from Fig. 1, the chargeneutrality line $n_p+n_d=2$, which corresponds to the compound LuNiBC, does not intersect any superconducting region. The electron–hole symmetry transformation $n_p\to 4-n_p$, $n_d\to 2-n_d$ transforms the chargeneutrality conditions into $\bar{n}_p+\bar{n}_d=5/2$ and $\bar{n}_p+\bar{n}_d=4$ for $Lu(NiB)_2C$ and LuNiBC, respectively. It can again be seen that in the electronic variables $\bar{n}_p$ and $\bar{n}_d$ the chargeneutrality line for LuNiBC does not pass through the superconductivity regions at all, while the line for $Lu(NiB)_2C$ passes through three superconducting regions. This is consistent with the experimentally observed lack of superconductivity in LuNiBC.

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