guish between the total energies $E_i(E_f)$ and the longitudinal energies $E_i^{\parallel}(E_f^{\parallel})$.

[4] The specific barrier height turns out to be unimportant for the levels considered.

[5] In Ref. 6 the quantity $J_{if}^{(1)}$ is given erroneously for this case.

[6] Integration over θ is carried out by elementary means in view of the presence of the δ function in Eq. (14).

[7] At high energies ($2E\varepsilon_i \gtrsim 1$) this spectrum is non-equidistant even for a parabolic well.

[1] D. S. Gemmell, Rev. Mod. Phys. **46**, 129 (1974).
[2] A. A. Vorobiev, V. V. Kaplin, and S. A. Vorobiev, Nucl. Instr. and Meth. **127**, 265 (1975).
[3] M. A. Kumakhov, Phys. Lett. **57A**, 17 (1976).
[4] M. A. Kumakhov, Zh. Eksp. Teor. Fiz. **72**, 1489 (1977) [Sov. Phys. JETP **45**, 781 (1977)].
[5] M. A. Kumakhov, Phys. Status Solidi B **84**, 41 (1977).
[6] V. A. Bazylev and N. K. Zhevago, Zh. Eksp. Teor. Fiz. **73**, 1697 (1977) [Sov. Phys. JETP **46**, 891 (1977)].
[7] E. A. Koptelov and N. P. Kalashnikov, Preprint, Nuclear Research Institute, Academy of Sciences, USSR, P-0054, 1977.
[8] V. V. Fedorov and A. I. Smirnov, Zh. Eksp. Teor. Fiz. **66**, 566 (1974) [Sov. Phys. JETP **39**, 271 (1974)].
[9] V. G. Baryshevskiĭ and I. Ya. Dubovskaya, Dokl. Akad. Nauk SSSR **231**, 1335 (1976) [Sov. Phys. Doklady **21**, 741 (1976)]; Phys. Status Solidi B **82**, 403 (1977).
[10] A. A. Vorob'ev, N. I. Zimin, and S. A. Vorob'ev, Izv. vuzov, seriya fiz. **8** (1977), Tomsk State University [Sov. Phys. Journal].
[11] R. W. Terhune and R. H. Pantell, Appl. Phys. Lett. **30**, 265 (1977).
[12] A. A. Sokolov and I. M. Ternov, Relyativistskiĭ élektron (The Relativistic Electron), Nauka, 1974.
[13] A. I. Akhiezer, V. F. Boldyshev, and N. F. Shul'ga, Preprint, Kharkov Physico-technical Institute, 77-38, 1977.
[14] B. R. Appleton, C. Erginsoy, and W. M. Gibson, Phys. Rev. **161**, 330 (1967).
[15] F. Fujimoto, S. Takagi, K. Komaki, H. Koike, and Y. Uchida, Radiat. Eff. **12**, 153 (1972).
[16] L. D. Landau and E. M. Lifshits, Kvantovaya mekhanika (Quantum Mechanics), Fizmatgiz, 1963.
[17] M. A. Kumakhov and R. Wedell, Phys. Status Solidi B **84**, 581 (1977).
[18] V. V. Beloshitskiĭ and M. A. Kumakhov, Dokl. Akad. Nauk SSSR **237**, 71 (1977) [Sov. Phys. Doklady **22**, 645 (1977)]. Zh. Eksp. Teor. Fiz. **74**, 1244 (1978) [Sov. Phys. JETP **47**, 652 (1978)].
[19] J. M. Ziman, Principles of the Theory of Solids, Cambridge University Press, Second Edition, 1972. Russ. transl., Mir, 1974.
[20] A. Edelyi, Ed., Higher Transcendental Functions, McGraw, 1953.
[21] V. S. Popov and A. M. Perelomov, Zh. Eksp. Teor. Fiz. **56**, 1375 (1969); **57**, 1684 (1969) [Sov. Phys. JETP **29**, 738 (1970); **30**, 910 (1970)].
[22] Yu. Kagan and Yu. V. Kononets, Zh. Eksp. Teor. Fiz. **58**, 226 (1970) [Sov. Phys. JETP **31**, 124 (1971)].
[23] D. F. Alferov, Yu. A. Bashmakov, and E. G. Bessonov, Trudy FIAN **80**, 100 (1975) [Proceedings of the P. N. Lebedev Physics Institute].

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Spin–orbit interaction in an excitonic dielectric

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The influence of spin–orbit interaction on the character of electron–hole pairing in a two-band model is considered. It is shown that the classification by the possible types of the ground state, given by Halperin and Rice [Solid State Physics, **21**, 115 (1968)], remains in force in this case. The degeneracy between the charge-current and spin-current states, which exists in the absence of spin–orbit interaction, is lifted. If the spin–orbit interaction is strong enough, the current state may turn out to be the ground state even in the absence of impurity scattering.

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1. INTRODUCTION

It is known that, depending on the phase of the order parameter and on its spin structure, four types of anomalous mean values are possible in electron–hole pairing.[1] It is shown in Ref. 2 that if no account is taken of the spin degree of freedom the system goes over into a state $\langle n(\mathbf{r})\rangle$, with a charge-density wave (ChDW) if the order parameter is real, and into a state $\langle \mathbf{j}(\mathbf{r})\rangle$ with a current-density wave (CuDW) if the order parameter is imaginary. If account is taken of the spin and of the associated choice of the sign of the order parameter Δ for opposite spin directions, then it can be seen that, depending on this choice, we get also a spin-density wave (SDW) $\langle \mathbf{S}(\mathbf{r})\rangle$, and for an imaginary order parameter we get a spin flux density wave (SFDW) $\langle \mathbf{S}(\mathbf{r})\mathbf{j}(\mathbf{r})\rangle$ for an imaginary order parameter. Each of these order parameters is characterized by its own effective coupling constant. Following Ref. 3, we can show that in the scheme of an isotropic semimetal, the effective coupling constants

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for the solution with real Δ corresponding to the charge and spin density waves are respectively

$$g_s=g_1+\tilde{g}_2+4(g_{ph}^2-g_2), \quad g_t=g_1+\tilde{g}_2. \tag{1}$$

At the same time, the constant for the solution with imaginary Δ, corresponding to solutions with current or spin flux density waves, is

$$g^{im}=g_1-\tilde{g}_2. \tag{2}$$

Here g_1 is the constant of an interaction of the density-density type, g_2 is the unrenormalized interaction connected with the transition of the pair from one band to another (of the type $g_2 a_1^+ a_1^+ a_2 a_2$), $\tilde{g}_2$ is the same screening-renormalized interaction, and g_{ph} is the value of the electron-phonon interband interaction. It is seen from (1) and (2) that the state with current and spin flux density waves is realized if electron-electron attraction exists in the interband channel, i.e., when

$$\tilde{g}_2<0, \quad \tilde{g}_2<2(g_2-g_{ph}^2). \tag{3}$$

Since the interaction with the constant g_2 is of short-lived character, g_2 and $\tilde{g}_2$ are practically equal. It appears therefore that the condition (3) cannot be realized, and the state with the current and with spin-flux density waves may turn out to be ground states only in the presence of interband impurity scattering.[2] This, as well as everything that follows, pertains equally well to the case of band extrema that coincide in momentum space, when the corresponding homogeneous states appear. It should be noted that regardless of the approximations (high density, etc.) in the exact equations for an arbitrary interaction force the symmetry and the character of the self-consistency equations remain unchanged, only the bare interaction is replaced by a complete interaction. Relation (2) indicates also that a state with imaginary Δ is degenerate.

All the foregoing dictates the aim of the present paper. It is, first, to investigate the influence of spin–orbit interaction on electron–hole pairing, to determine how the states with real and imaginary order parameters vary, and what conditions are necessary in place of (3) to realize the current state as a ground state. Second, we wish to show how the degeneracy, with respect to the states with the current and spin-flux density waves, is lifted for the principal solution with the minimum order parameter, which follows from the equality of the effective coupling constants for the states with the current and spin-flux charge densities, without the spin–orbit interaction.

For simplicity we solve the problem for an isotropic semimetal whose crystal lattice has an inversion center. We note that all the conclusions obtained for this model remain in force for semiconductors with narrow forbidden bands. All this is intended only to facilitate the calculations. To eliminate the computational difficulties, we shall exclude the interband electron–phonon interactions from the system Hamiltonian, and also neglect the renormalization of g_2 in the exchange diagrams due to screening of the interaction.

2. HAMILTONIAN OF THE SYSTEM

We divide the Hamiltonian $\hat{H}$ of our system into three parts: $\hat{H}_0, \hat{H}_{int}^{(1)}$ and $\hat{H}_{int}^{(2)}$, where $\hat{H}_0$ is of the Hamiltonian of the electrons that do not interact with one another and are located in the periodic field of the lattice; $\hat{H}_{int}^{(1)}$ is the part of the electron–electron Hamiltonian in which are left only the terms responsible for the exciton instability of the density–density type for electrons from different bands, and the terms that take into account the transitions of the electrons from one band into another without spin flip. Finally, $\hat{H}_{int}^{(2)}$ is the second part of the Hamiltonian of the electron–electron interaction, whose terms correspond to the transition of electrons of one band into another with spin flip. We note that in the one-particle Hamiltonian we did not include in explicit form the spin–orbit interaction, since this interaction does not spin-split the spectrum of crystals with inversion centers. The effect of this interaction on the electron–hole pairing is investigated with the aid of the generalized Bloch functions.

In the presence of spin–orbit interaction, the zeroth-Hamiltonian wave eigenfunctions are of the Bloch type and are spinors. In the general case

$$\varphi_{k\uparrow}(\mathbf{r})=\begin{pmatrix} u_k(\mathbf{r}) \\ v_k(\mathbf{r}) \end{pmatrix} e^{i\mathbf{kr}}, \tag{4}$$

where the arrows in the subscripts of the Bloch functions $\varphi_{k\uparrow}$ and $\varphi_{k\downarrow}$ indicate the spin state: for example, in the former case the spin is directed in general upward in the sense that the mean value $(\varphi_{k\uparrow}, \sigma_z \varphi_{k\uparrow}$ is positive. In the presence of spin–orbit interaction, the functions $u_k(\mathbf{r})$ and $v_k(\mathbf{r})$ satisfy the equations

$$\left(\frac{1}{2m}(\hat{\mathbf{p}}+\mathbf{k})^2+V(\mathbf{r})+\frac{1}{4m^2c^2}[\boldsymbol{\sigma}\times\operatorname{grad}V(\mathbf{r})](\hat{\mathbf{p}}+\mathbf{k})\right) \times\begin{pmatrix} u_k(\mathbf{r}) \\ v_k(\mathbf{r}) \end{pmatrix}=\varepsilon_k\begin{pmatrix} u_k(\mathbf{r}) \\ v_k(\mathbf{r}) \end{pmatrix}. \tag{5}$$

Here $\hat{\mathbf{p}}$ is an operator, $\mathbf{k}$ is a number, and $V(\mathbf{r})$ is the periodic potential of the crystal lattice. It is seen from these equations that $u_k(\mathbf{r})$ differs from $v_k(\mathbf{r})$.

Since the Hamiltonian is invariant to the space inversion operation I, we have accurate to a phase factor

$$\varphi_{k\uparrow}(\mathbf{r})=\varphi_{-k\uparrow}(-\mathbf{r}), \quad \varepsilon_{k\uparrow}=\varepsilon_{-k\uparrow}. \tag{6}$$

In addition, from the invariance of the Hamiltonian to time reversal, it follows that

$$\varphi_{k\downarrow}=KI\varphi_{k\uparrow}, \quad \varepsilon_{k\uparrow}=\varepsilon_{k\downarrow}, \tag{7}$$

where $K=-i\sigma_y K_0$ is the time-reversal operator according to Kramers, K_0 is the operation of complex conjugation, and σ_y is a Pauli matrix. Relations (7) show that for crystals with inversion center the spin degeneracy is not lifted, a fact we already noted earlier.

Regarding from the very beginning $u_k(\mathbf{r})$ and $v_k(\mathbf{r})$ as real functions, something also possible for band extrema, we obtain also an expression for $\varphi_{k\downarrow}$ in terms of these functions:

$$\varphi_{k_1}(\mathbf{r})=\begin{pmatrix}-v_k(\mathbf{r})\\ u_k(\mathbf{r})\end{pmatrix}\exp(i\mathbf{kr}). \tag{8}$$

We note that complex $u_k(\mathbf{r})$ and $v_k(\mathbf{r})$ yield no new qualitative changes.

We continue the analysis of the problem in the high-density approximation (this does not change the results qualitatively), when the following inequality is satisfied

$$|\mathscr{E}_g|\gg e^2\varkappa/\varepsilon, \tag{9}$$

where $\mathscr{E}_g$ is the width of the forbidden band and is negative ($\mathscr{E}_g<0$) for a semimetal, e is the electron charge, ε is the dielectric constant of the lattice, and $\varkappa$ is the reciprocal screening radius. In this case the effective interaction potentials can be replaced by momentum-independent constants.

The single-particle Hamiltonian of the isotropic semimetal is of the form

$$\hat{H}_0=\sum_{\mathbf{k},\alpha}\left(\frac{\hbar^2\mathbf{k}^2}{2m}+\frac{\mathscr{E}_g}{2}\right)(a_{1\alpha}^+(\mathbf{k})a_{1\alpha}(\mathbf{k})-a_{2\alpha}^+(\mathbf{k})a_{2\alpha}(\mathbf{k})). \tag{10}$$

Here $\hbar\mathbf{k}$ is the quasimomentum of the electron, 1 and 2 are the indices of the conduction and valence bands, respectively, m is the effective mass, which for simplicity is assumed to the same for electrons ahd holes, and $a_{1\alpha}(\mathbf{k})$, $a_{2\alpha}(\mathbf{k})$ are the fermion operators of electron annihilation in bands 1 and 2, respectively, in states of the type (4) and (8).

We have similarly expressions for $\hat{H}_{\text{int}}^{(1)}$ and $\hat{H}_{\text{int}}^{(2)}$:

$$\begin{aligned}\hat{H}_{int}^{(1)}=\sum_{\substack{\mathbf{k},\mathbf{k}',\\ \alpha,\beta}}\{&g_1a_{1\alpha}^+(\mathbf{k})a_{2\beta}^+(\mathbf{k}')a_{2\beta}(\mathbf{k}')a_{1\alpha}(\mathbf{k})\\ &+g_2[a_{1\alpha}^+(\mathbf{k})a_{1\beta}^+(\mathbf{k}')a_{2\beta}(\mathbf{k}')a_{2\alpha}(\mathbf{k})\\ &+a_{1\alpha}^+(\mathbf{k})a_{2\beta}^+(\mathbf{k}')a_{1\beta}(\mathbf{k}')a_{2\alpha}(\mathbf{k})+\text{h.c.}]\},\end{aligned} \tag{11}$$

$$\begin{aligned}\hat{H}_{int}^{(2)}=\sum_{\substack{\mathbf{k},\mathbf{k}',\\ \alpha\neq\beta}}\{&g_2'[a_{1\alpha}^+(\mathbf{k})a_{1\alpha}^+(\mathbf{k}')a_{2\beta}(\mathbf{k}')a_{2\beta}(\mathbf{k})\\ &-a_{1\alpha}^+(\mathbf{k})a_{2\alpha}^+(\mathbf{k}')a_{1\beta}(\mathbf{k}')a_{2\beta}(\mathbf{k})+a_{1\alpha}^+(\mathbf{k})a_{2\beta}^+(\mathbf{k}')a_{1\alpha}(\mathbf{k}')a_{2\beta}(\mathbf{k})\\ &-a_{1\alpha}^+(\mathbf{k})a_{1\beta}^+(\mathbf{k}')a_{2\alpha}(\mathbf{k}')a_{2\beta}(\mathbf{k})+\text{h.c.}]\\ &+g_2''[\alpha(a_{1\alpha}^+(\mathbf{k})a_{1\beta}^+(\mathbf{k}')a_{2\beta}(\mathbf{k}')a_{2\beta}(\mathbf{k})\\ &+a_{1\alpha}^+(\mathbf{k})a_{1\alpha}^+(\mathbf{k}')a_{2\alpha}(\mathbf{k}')a_{2\beta}(\mathbf{k})-\text{h.c.})\\ &+\alpha(a_{1\alpha}^+(\mathbf{k})a_{2\beta}^+(\mathbf{k}')a_{1\beta}(\mathbf{k}')a_{2\beta}(\mathbf{k})\\ &+a_{1\beta}^+(\mathbf{k})a_{2\beta}^+(\mathbf{k}')a_{1\alpha}(\mathbf{k}')a_{2\alpha}(\mathbf{k})+\text{h.c.})]\}.\end{aligned} \tag{12}$$

Here g_1 and g_2 were defined above, g_2' is the bare interaction connected with the transition of a pair of electrons from one band to another, when both electrons change the spin direction in the transition, and g_2'' is the same bare interaction, but when the spin of one of the electrons is reversed in the transition (we have in mind the generalized spin). We note that the values of g_2, g_2', and g_2'' are different and are determined by the formulas

$$\begin{aligned}g_2&=\iint\varphi_{1\alpha}^*(\mathbf{r})\varphi_{1\beta}^*(\mathbf{r}')V_c(\mathbf{r}-\mathbf{r}')\varphi_{2\beta}(\mathbf{r}')\varphi_{2\alpha}(\mathbf{r})\,d\mathbf{r}\,d\mathbf{r}',\\ g_2'&=\iint\varphi_{1\alpha}^*(\mathbf{r})\varphi_{1\alpha}^*(\mathbf{r}')V_c(\mathbf{r}-\mathbf{r}')\varphi_{2\beta}(\mathbf{r}')\varphi_{2\beta}(\mathbf{r})\,d\mathbf{r}\,d\mathbf{r}',\\ g_2''&=\iint\varphi_{1\alpha}^*(\mathbf{r})\varphi_{1\beta}^*(\mathbf{r}')V_c(\mathbf{r}-\mathbf{r}')\varphi_{2\beta}(\mathbf{r}')\varphi_{2\beta}(\mathbf{r})\,d\mathbf{r}\,d\mathbf{r}',\end{aligned} \tag{13}$$

where $V_c(\mathbf{r}-\mathbf{r}')$ is the Coulomb interaction; in the foregoing formulas $\alpha\neq\beta$ and to simplify the notation we have left out the k indices.

With the aid of (4), (8), and the expressions for g_2, g_2', and g_2'' it is easily seen that all the terms in $\hat{H}_{\text{int}}^{(1)}$ should enter with a plus sign, while the sign in $\hat{H}_{\text{int}}^{(2)}$ alternates, depending on the direction of the electron spins.

Thus, the total Hamiltonian of the investigated system is of the form

$$\hat{H}=\hat{H}_0+\hat{H}_{int}^{(1)}+\hat{H}_{int}^{(2)}. \tag{14}$$

3. SELF-CONSISTENT SYSTEM OF FUNDAMENTAL EQUATIONS

The system described by the Hamiltonian (14) is analyzed with the aid of a diagram technique for time-dependent Green's functions.[4] The Green's function is defined by

$$G_{\alpha,\beta}(\mathbf{r},\mathbf{r}')=-i\langle T\psi_\alpha(\mathbf{r},t)\psi_\beta^+(\mathbf{r}',0)\rangle, \tag{15}$$

where $\psi_\alpha(\mathbf{r},t)$, $\psi_\alpha^*(\mathbf{r},t)$ are the operators of annihilation and creation of an electron at the point $\mathbf{r}$ with generalized spin $\alpha/2$ in the Heisenberg representation. In the Schrödinger representation these operators can be expressed in terms of the electron creation and annihilation operators $a_{i\alpha}^+(\mathbf{k})$, $a_{i\alpha}(\mathbf{k})$ with quasimomentum $\hbar\mathbf{k}$. In the two-band model we have

$$\begin{aligned}\psi_\alpha(\mathbf{r})&\approx\sum_{\mathbf{k}}\{\varphi_{1\mathbf{k}\alpha}(\mathbf{r})a_{1\alpha}(\mathbf{k})+\varphi_{2\mathbf{k}\alpha}(\mathbf{r})a_{2\alpha}(\mathbf{k})\},\\ \psi_\alpha^+(\mathbf{r})&\approx\sum_{\mathbf{k}}\{\dot{\varphi}_{1\mathbf{k}\alpha}(\mathbf{r})a_{1\alpha}^+(\mathbf{k})+\dot{\varphi}_{2\mathbf{k}\alpha}(\mathbf{r})a_{2\alpha}^+(\mathbf{k})\},\end{aligned} \tag{16}$$

where $\varphi_{i\mathbf{k}\alpha}$ are the generalized Bloch functions introduced above, with electron quasimomentum $\hbar\mathbf{k}$, in the electron and hole bands. We change over to the matrix element of the total Green's function (15), calculated in the generalized basis of the Bloch functions:

$$G_{ij}^{\alpha\beta}(\mathbf{k},t)=-i\langle Ta_{i\alpha}(\mathbf{k})a_{j\beta}^+(\mathbf{k})\rangle; \tag{17}$$

Here i and j are the band indices.

The time-dependent Fourier components of the zeroth Green's functions are of the usual form

$$\begin{aligned}G_1^{(0)}(\mathbf{k},\omega)&=[\omega+\hbar^2\mathbf{k}^2/2m+\mathscr{E}_g/2]^{-1},\\ G_2^{(0)}(\mathbf{k},\omega)&=[\omega-\hbar^2\mathbf{k}^2/2m-\mathscr{E}_g/2]^{-1}.\end{aligned} \tag{18}$$

We write down also the expression for the total Green's function in terms of its matrix elements (17):

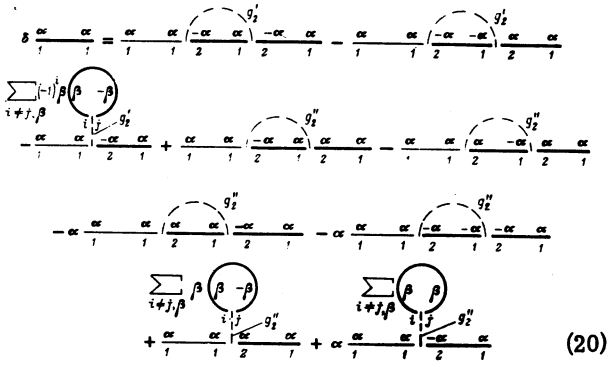
$$G_{\alpha\beta}(\mathbf{r},\mathbf{r}';t)=\sum_{i,j,\mathbf{k}}G_{ij}^{\alpha\beta}(\mathbf{k},t)\dot{\varphi}_{j\mathbf{k}\beta}(\mathbf{r}')\varphi_{i\mathbf{k}\alpha}(\mathbf{r}). \tag{19}$$

The total Green's function will be represented on the diagrams by a thick line, with the band indices marked below the line and the spin indices above the line. The free Green's functions $G_1^{(0)}(\mathbf{k},t)$ and $G_2^{(0)}(\mathbf{k},t)$, which correspond to the Hamiltonian (10), are diagonal in the band and in the spin indices; they are represented by

a thin solid line. We note, in the case of high density (9), to find the anomalous Green's function, it suffices to retain in the corresponding equations only the direct and exchange diagrams, which contain the interband Green's functions $G_{ij}^{\alpha\beta}$ at $i \neq j$. This corresponds to the Hartree–Fock approximation.

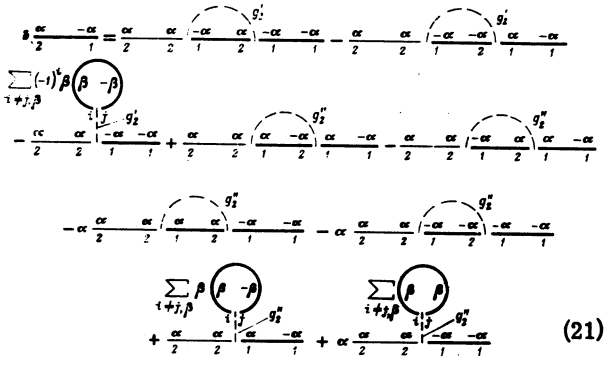
The diagrams obtained from $H_{\text{int}}^{(1)}$ and the corresponding analytic expressions for the Green's functions coincide with those obtained in Ref. 3, and we therefore write out only the corresponding analytic expressions. Using the notation given above, we write down those additional digrams which are obtained from $H_{\text{int}}^{(2)}$, denoting the additional part of the Green's function by $\delta G_{ij}^{\alpha\beta}$.

The diagrams for $\delta G_{11}^{\alpha\alpha}$ are:



(20)

The diagrams for $\delta G_{21}^{\alpha,-\alpha}$ are:



(21)

The letters α and β in front of the diagrams indicate the sign. For example, for δG_{11}^{11} a plus sign in front of the last diagram remains a plus sign, while in the case of δG_{11}^{-11} it changes to a minus sign. In analytic form, the expressions for the Green's functions are

$$G_{11}^{\alpha\alpha}(\mathbf{k},\omega)=G_1^{(0)}(\mathbf{k},\omega)-iG_1^{(0)}(\mathbf{k},\omega)\Big\{\sum_{\mathbf{k}',\omega'}[g_1G_{12}^{\alpha\alpha}+g_2G_{21}^{\alpha\alpha}]$$
$$-\sum_{\mathbf{k}',\omega',\beta}g_2[G_{21}^{\beta\beta}+G_{12}^{\beta\beta}]-\sum_{\mathbf{k}',\omega'}g_2'G_{21}^{-\alpha,-\alpha}$$
$$+\alpha\sum_{\mathbf{k}',\omega'}g_2''[G_{12}^{-\alpha\alpha}-G_{12}^{\alpha,-\alpha}]\Big\}G_{21}^{\alpha\alpha}(\mathbf{k},\omega)$$
$$-iG_1^{(0)}(\mathbf{k},\omega)\Big\{\sum_{\mathbf{k}',\omega'}[g_1G_{12}^{\alpha,-\alpha}+g_2G_{21}^{\alpha,-\alpha}]+\sum_{\mathbf{k}',\omega'}g_2'[G_{21}^{\alpha,-\alpha}-G_{12}^{\alpha,-\alpha}+G_{12}^{-\alpha,\alpha}]$$
$$-\alpha\sum_{\mathbf{k}',\omega',\beta}g_2''G_{12}^{\beta\beta}\Big\}G_{21}\quad(\mathbf{k},\omega). \tag{22}$$

We note that all the Green's functions under the summation sign depend on $\mathbf{k}'$ and ω'. Equations for $G_{11}^{\alpha,-\alpha}$, $G_{21}^{\alpha\alpha}$, $G_{21}^{\alpha,-\alpha}$ are written in similar form.

It should be noted, as indicated in Ref. 3, that Eq. (22) is gauge-invariant because it includes terms that contain the coupling constants g_2, g_2', and g_2'' and also Hartree terms. Therefore it is not contradictory in two cases: for pure real and pure imaginary phase factors for the interband Green's function.

For the matrices $G_{11}^{\alpha\beta}(\mathbf{k},\omega)$ and $G_{21}^{\alpha\beta}(\mathbf{k},\omega)$ over the spin indices α and β we can write down a system of equations in matrix form:

$$(\omega-\xi(\mathbf{k}))\hat{G}_{11}=I+\hat{\Delta}\hat{G}_{21},\quad(\omega+\xi(\mathbf{k}))\hat{G}_{21}=\hat{\Delta}+\hat{G}_{11}, \tag{23}$$

where $\xi(\mathbf{k})=\hbar^2k^2/2m+\mathscr{E}_g/2$, I is a unit two-dimensional matrix, and $\hat{\Delta}$ is the matrix of the order parameter.

We consider now separately solutions with real and imaginary order parameters.

A. States with real Δ

For the components of the order-parameter matrix $\hat{\Delta}$ we can obtain the system of self-consistency equations

$$\Delta_{11}+\Delta_{-1,-1}=(g_1-3g_2-g_2')(\Delta_{11}+\Delta_{-1,-1})K-2g_2''(\Delta_{1,-1}-\Delta_{-11})K,$$
$$\Delta_{11}-\Delta_{-1,-1}=(g_1+g_2+g_2')(\Delta_{11}-\Delta_{-1,-1})M,$$
$$\Delta_{1,-1}+\Delta_{-1,1}=(g_1+g_2+g_2')(\Delta_{1,-1}+\Delta_{-1,1})M,$$
$$\Delta_{1,-1}-\Delta_{-1,1}=(g_1+g_2-g_2')(\Delta_{1,-1}-\Delta_{-1,1})K-2g_2''(\Delta_{11}+\Delta_{-1,-1})K,$$
$$K=-i\sum_{\mathbf{k},\omega}\frac{\omega^2-\xi^2(\mathbf{k})-(\Delta_{11}\Delta_{-1,-1}-\Delta_{1,-1}\Delta_{-1,1})}{\text{Det}},$$
$$M=-i\sum_{\mathbf{k},\omega}\frac{\omega^2-\xi^2(\mathbf{k})+(\Delta_{11}\Delta_{-1,-1}-\Delta_{1,-1}\Delta_{-1,1})}{\text{Det}}. \tag{24}$$

The symbol Det stands for an expression that determines the spectrum of the single-particle excitations:

$$\text{Det}=[\omega^2-\xi^2(\mathbf{k})]^2-(\omega^2-\xi^2(\mathbf{k}))(\Delta_{11}^2+\Delta_{-1,-1}^2$$
$$+\Delta_{1,-1}^2+\Delta_{-1,1}^2)+(\Delta_{11}\Delta_{-1,-1}-\Delta_{1,-1}\Delta_{-1,1})^2. \tag{25}$$

It is seen from the obtained system (24) that when $g_2'=g_2''=0$ we have the self-consistency conditions for the singlet (Δ_s^0) and triplet (Δ_t^0) order parameters[5]:

$$\Delta_s^0=-i\frac{g_s}{2}\sum_{\mathbf{k},\omega}\text{Sp}\,\hat{G}_{21},\quad\Delta_t^0=-i\frac{g_t}{2}\sum_{\mathbf{k},\omega}\text{Sp}\,\sigma\hat{G}_{21}.$$

The second and third equations yield Δ_t^{0x}, Δ_t^{0x} and the fourth equation multiplied by i yields Δ_t^{0y}.

The system (24) can be reduced to two equations relative to the new unknowns Δ_s and Δ_t defined by the relations

$$(\Delta_{11}+\Delta_{-1,-1})\left[2\left(1+\frac{g_2}{(g_2^2+g_2''^2)^{1/2}}\right)\right]^{-1/2}=\Delta_s,$$
$$(\Delta_{11}-\Delta_{-1,-1})/2=\Delta_t \tag{26}$$

under the additional condition that follows from (24):

$$\Delta_{1,-1}-\Delta_{-11}=\frac{g_2''}{g_2+(g_2^2+g_2''^2)^{1/2}}(\Delta_{11}+\Delta_{-1,-1}),\quad\Delta_{1,-1}=-\Delta_{-1,1}, \tag{27}$$

The singlet and triplet coupling constants are deter-

mined as follows:

$$g_s=g_1-g_2-g_2'-2(g_2^2+g_2''^2)^{1/2}, \quad g_t=g_1+g_2+g_2'. \tag{28}$$

If we substitute in (26) $g_2'=g_2''=0$, then at $g_2>0$ we obtain $g_s=g_1-3g_2$, which agrees with the known results obtained in Ref. 3, but at $g_2<0$ we have $g_s=g_t|g_2|$, which corresponds to the maximum energy. This indicates that at $g_2<0$ we should take the second root of K.

We note that the system consisting of the first and fourth equations of (24) has nonzero solutions when their determinant is equal to zero. It is the vanishing of this determinant which gives two roots for K: the root

$$K_1=[g_1-g_2-g_2'-2(g_2^2+g_2''^2)^{1/2}]^{-1},$$

which was used above, and

$$K_2=[g_1-g_2-g_2'+2(g_2^2+g_2''^2)^{1/2}]^{-1}.$$

Using the second root K_2 we determine the constants g_s and g_t at $g_2<0$ in the following manner:

$$g_s=g_1-g_2-g_2'+2(g_2^2+g_2''^2)^{1/2}, \quad g_t=g_1+g_2+g_2' \tag{28a}$$

and corresponding new relations that connect the old unknowns with the new ones:

$$(\Delta_{11}+\Delta_{-1,-1})\left[2\left(1-\frac{g_2}{(g_2^2+g_2''^2)^{1/2}}\right)\right]^{-1/2}=\Delta_s, \quad \frac{\Delta_{11}-\Delta_{-1,-1}}{2}=\Delta_t, \tag{26a}$$

$$\Delta_{1,-1}-\Delta_{-1,1}=\frac{g_2''}{g_2-(g_2^2+g_2''^2)^{1/2}}(\Delta_{11}+\Delta_{-1,-1}), \quad \Delta_{1,-1}=-\Delta_{-1,1}. \tag{27a}$$

Relative to the new unknowns Δ_s and Δ_t, the system of two equations coincides with that obtained in Ref. 3.

It remains to make sure that the quantities Δ_s and Δ_t given by (26) or (26a) actually correspond to states with charge density and spin density waves. To this end we calculate the local charge density $Q(\mathbf{R})=\langle n(\mathbf{R})\rangle$ and the local magnetic moment $\mathbf{M}(\mathbf{R})=\langle \mathbf{S}(\mathbf{R})\rangle$. The matrices of the corresponding operators are given by

$$\hat{n}(\mathbf{R})=el\delta(\mathbf{r}-\mathbf{R}), \quad \hat{\mathbf{S}}(\mathbf{R})=m_B\sigma_{\alpha,\beta}\delta(\mathbf{r}-\mathbf{R}), \tag{29}$$

and with the aid of these operators we obtain expressions for $Q(R)$ and $\mathbf{M}(R)$:

$$\begin{aligned} Q(\mathbf{R})&=-ie\sum_{i,j,\mathbf{k}}\mathrm{Sp}\,\hat{A}_{ij}(\mathbf{R};\mathbf{k},-0),\\ \mathbf{M}(\mathbf{R})&=-im_B\sum_{i,j,\mathbf{k}}\mathrm{Sp}[\sigma\hat{A}_{ij}(\mathbf{R};\mathbf{k},-0)], \end{aligned} \tag{30}$$

where the matrix $\hat{A}_{ij}(\mathbf{R};\mathbf{k},-0)$ has matrix elements of the type

$$\varphi_{i\mathbf{k}\alpha}(\mathbf{R})\varphi^*_{j\mathbf{k}\beta}(\mathbf{R})G_{ij}^{\alpha\beta}(\mathbf{k},-0).$$

After rather simple calculations we obtain

$$\begin{aligned} Q(\mathbf{R})&=2eQ_{12}(\mathbf{R})\frac{\Delta_s}{g_s}\left[2\left(1\pm\frac{g_2}{(g_2^2+g_2''^2)^{1/2}}\right)\right]^{1/2},\\ M_z(\mathbf{R})&=2m_BQ_{12}(\mathbf{R})\frac{2\Delta_t}{g_t}, \end{aligned} \tag{30a}$$

where $Q_{12}(\mathbf{R})$ is the matrix element of the operator $\hat{n}(\mathbf{R})$. The obtained expressions indicate that Δ_s and Δ_t indeed correspond to states with charge density and spin density waves, respectively.

B. States with imaginary order parameter

As already stated, the matrix of the order parameter $\hat{\Delta}$ can be either real or imaginary. States with real $\hat{\Delta}$ were investigated above. We investigated here the case of an imaginary order parameter. An imaginary order parameter is obtained if $G_{21}^{\alpha\beta}$ in the system (23) has an imaginary phase factor. For the components of the matrix of the order parameter $\hat{\Delta}$ we have the following self-consistency conditions:

$$\begin{aligned} \Delta_{11}+\Delta_{-1,-1}&=(g_1-g_2+g_2')(\Delta_{11}+\Delta_{-1,-1})K-2g_2''(\Delta_{1,-1}-\Delta_{-11})K,\\ \Delta_{11}-\Delta_{-1,-1}&=(g_1-g_2-g_2')(\Delta_{11}-\Delta_{-1,-1})M,\\ \Delta_{1,-1}+\Delta_{-1,1}&=(g_1-g_2-g_2')(\Delta_{1,-1}+\Delta_{-1,1})M,\\ \Delta_{1,-1}-\Delta_{-1,1}&=(g_1-g_2-3g_2')(\Delta_{1,-1}-\Delta_{-1,1})K-2g_2''(\Delta_{11}+\Delta_{-1,-1})K. \end{aligned} \tag{31}$$

The expressions for K and M are the same as in the system (24). We note that the system (31) contains the moduli of the components of the imaginary matrix $\hat{\Delta}$.

The system (31) reduces analogously to two equations with respect to new unknowns Δ_s^{im} and Δ_t^{im}, defined by the relations

$$\begin{aligned} (\Delta_{11}+\Delta_{-1,-1})\left[2\left(1+\frac{g_2'}{(g_2'^2+g_2''^2)^{1/2}}\right)\right]^{-1/2}&=\Delta_s^{im},\\ \frac{\Delta_{11}-\Delta_{-1,-1}}{2}&=\Delta_t^{im}, \end{aligned} \tag{32}$$

subject to an additional condition analogous to (25):

$$\begin{aligned} \Delta_{1,-1}-\Delta_{-1,1}&=-\frac{g_2''}{g_2'+(g_2'^2+g_2''^2)^{1/2}}(\Delta_{11}+\Delta_{-1,-1}),\\ \Delta_{1,-1}&=-\Delta_{-1,1}. \end{aligned} \tag{33}$$

The singlet and triplet coupling constants take the form

$$g_s^{im}=g_1-g_2-g_2'+2(g_2'^2+g_2''^2)^{1/2}, \quad g_t^{im}=g_1-g_2-g_2'. \tag{34}$$

We note that for K_1, just as in the case A, we obtain one more root, but we choose the first of them, which corresponds to the minimum energy.

The new system of equations with respect to Δ_s^{im} and Δ_t^{im} also corresponds with the system obtained in Ref. 3. Starting from the expressions for the current density and the spin-flux density[1]

$$\begin{aligned} \mathbf{j}(\mathbf{R})&=\frac{e\hbar}{2mi}\sum_{\alpha}[\psi_\alpha^+\times(\mathbf{R})\nabla\psi_\alpha(\mathbf{R})-[\nabla\psi_\alpha^+(\mathbf{R})]\psi_\alpha(\mathbf{R})],\\ \mathbf{j}^s(\mathbf{R})&=\frac{e\hbar}{2mi}\sum_{\alpha,\beta}[\psi_\alpha^+\times(\mathbf{R})\nabla\psi_\beta(\mathbf{R})-[\nabla\psi_\alpha^+(\mathbf{R})]\psi_\beta(\mathbf{R})]\sigma_{\alpha\beta}, \end{aligned} \tag{35}$$

we obtain

$$\begin{aligned} \mathbf{j}(\mathbf{R})&=\frac{e\hbar\mathbf{I}_{12}(\mathbf{R})}{m}\frac{\Delta_s^{im}}{g_s^{im}}\left[2\left(1+\frac{g_2'}{(g_2'^2+g_2''^2)^{1/2}}\right)\right]^{1/2},\\ j^s(\mathbf{R})&=\frac{e\hbar\mathbf{I}_{12}(\mathbf{R})}{m}\frac{2\Delta_t^{im}}{g_t^{im}}. \end{aligned} \tag{36}$$

The expressions for the current density and the spin-flux density indicate that Δ_s^{im} and Δ_t^{im} indeed correspond to respective states with current and spin-flux density waves.

4. CONCLUSIONS

Allowance for the spin-orbit interaction leads to a substantial renormalization of the effective coupling constants. This renormalization makes it possible to obtain less stringent conditions for the realization of the current states than the conditions (3) (just as above with the electron-phonon interaction neglected). We examine the cases $g_2<0$ and $g_2>0$ separately.

1) $g_2<0$. In this case the state with the current charge density is more convenient if a) $|g_2|<|g_2'|$ at $g_2'<0$; b) $(g_2'^2+g_2''^2)^{1/2}>g_2'-|g_2|$ at $g_2'>0$.

2) $g_2>0$. In this case we have for the realization of the current states the following conditions: c) $(g_2'^2+g_2''^2)^{1/2}>(g_2+g_2')$ at $g_2'>0$ and d) $(g_2'^2+g_2''^2)^{1/2}>(g_2-|g_2'|)$ at $g_2'<0$.

It is seen that the more favorable conditions are b) and d), which require only that $g_2g_2'<0$ and that their difference be small. The case b) corresponds to attraction in the interband channel between electrons having like spin, and repulsion of electrons having unlike spin, while the case d) corresponds to repulsion of electrons with like spin direction in the interband channel and attraction of electrons with different spin directions.

Thus, from a comparison of expressions (28), (28a), and (34), it is seen that for a sufficiently strong spin-orbit interaction the state with the current density wave may turn out to be the ground state even in the absence of impurity scattering.[2] Equally well, as from (32), the degeneracy between the state with the current density wave and the state with the spin flux density wave, which is present if there is no spin-orbit interaction ($g_2'=g_2''=0$), is lifted by this interaction, the state with the current density wave being favored in this case.

The most unexpected result of the present analysis is the following. With increasing spin-orbit interaction, the spin ceases to be a good quantum number. One can therefore hope that, for example, states with charge density waves and spin density waves, which are characterized in the absence of spin-orbit interaction by singlet and triplet spin structures of the electron-hole pairs, become entangled, i.e., a state is possible in which the charge and spin density waves exist simultaneously. However, the foregoing analysis of the self-consistency equations for Δ shows that the stationary structures are those corresponding either to charge density waves or spin density waves (see (30a)). The coexistence of the spin and charge density waves, which leads to a ferromagnetic state, is possible only if the electron and hole Fermi surfaces are not fully congruent, as well as in the absence of spin-orbit interaction.[3]

Similar reasoning can be applied also to states with current and spin-density waves.

All the results presented in this paper remain unchanged if the extrema of the bands coincide in momentum space. Instead of the charge density wave we get here a shift of the sublattices and ferroelectric ordering if the matrix element of the momentum operator differs from zero.[6]

A state with spin density wave will have the period of the initial crystal lattice. Instead of the states with current and spin–flux density waves there will occur corresponding homogeneous current states[1] if the magnetic field of these currents is not taken into account.

[1]B. I. Halperin and T. M. Rice, Solid State Phys. 21, 115 (1968).

[2]B. A. Volkov and Yu. V. Kopaev, Pis'ma Zh. Eksp. Teor. Fiz. 27, 10 (1978) [JETP Lett. 27, 7 (1978)].

[3]B. A. Volkov, Yu. V. Kopaev, and A. I. Rusinov, Zh. Eksp. Teor. Fiz. 68, 1899 (1975) [Sov. Phys. JETP 41, 952 (1975)].

[4]A. A. Abrikosov, L. P. Gor'kov, and I. E. Dzyaloshinskiĭ, Metody kvantovoĭ teorii polya v statisticheskoĭ fizike (Quantum Field Theoretical Methods in Statistical Physics), Fizmatgiz, 1962 [Pergamon, 1965].

[5]B. A. Volkov, A. I. Rusinov, and R. Kh. Timerov, Zh. Eksp. Teor. Fiz. 70, 1130 (1976) [Sov. Phys. JETP 43, 589 (1976)].

[6]V. M. Elesin and Yu. V. Kopaev, Pis'ma Zh. Eksp. Teor. Fiz. 24, 78 (1976) [JETP Lett. 24, 66 (1976)].

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