Paramagnetic limit of superconductors with dielectric gap on the Fermi surface

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The magnetic properties of a superconductor with degenerate electron spectrum are considered. It is shown that the upper critical magnetic field H_{c2} of a superconductor with a dielectric gap Σ on the Fermi surface can exceed the Clogston-Chandrasekhar paramagnetic limit.

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1. INTRODUCTION

Many type-II superconductors were recently discovered with relatively low critical temperatures T_c and with upper critical fields $H_{c2}(0)$ greatly exceeding the paramagnetic limit $H_{p0}=(\pi/\gamma)T_c/\mu_B\sqrt{2}\approx 18,4T_c$ [kG], where μ_B is the Bohr magneton and $\gamma=1.78\dots$ is the Euler constant (see Refs. 1–6). This phenomenon can be due to various causes, for example: the onset of an inhomogeneous superconducting Fulde-Ferell-Larkin-Ovchinnikov state,[7] spin-orbit scattering of electrons by impurities,[8] spin-orbit interaction in crystals without inversion center,[9] compensation of the external magnetic field by an internal volume field,[10] triplet pairing of electrons in layered compounds[11] and in crystals with giant Kohn anomaly,[12] and the suppression of spin fluctuations (paramagnons) in strong magnetic fields.[13] In addition, the apparent exceeding of the paramagnetic limit can be observed in superconductors with strong electron-phonon coupling, for which the Bardeen-Cooper-Schrieffer (BCS) relation between T_c and the superconducting gap Δ_0 at $T=0$ is not satisfied,[14] so that $\Delta_0>\pi T_c/\gamma$ and the Clogston-Chandrasekhar limit $H_p\equiv\Delta_0/\mu_B\sqrt{2}>H_{p0}$.

Yet a common property of superconducting compounds in which the paramagnetic limit is seen to be exceeded is an instability to the formation of a dielectric gap on the Fermi surface (FS). Thus, a structural instability accompanied by partial dielectrization of the electron spectrum takes place in layered dichalgonides of transition metals,[4] in compounds with C15 structure (Laves phases)[15-18] and in ternary modybdenum chalcogenides (Chevrel phases).[19-21] As to the inorganic polymer $(SN)_x$, here, too one cannot exclude the possible existence of a very small dielectric gap on the FS, since the temperature dependence of its resistivity has a characteristic minimum[22] and is analogous to the $\rho(T)$ for the organic metal HMTSeF–TCNQ,[23] in which charge density waves (CDW) were observed up to room temperatures,[24] apparently due to Peierls instability.

It is shown in the present paper that the onset of the dielectric gap of collective character on the FS can greatly increase the paramagnetic limit of the superconductor in the case of either complete of partial dielectrization of the electron spectrum. This situation arises if the FS has section with a degenerate spectrum of the form $\varepsilon(\mathbf{p})=-\varepsilon(\mathbf{p}+\mathbf{q})$, which is typical of semimetals and metals with narrow conduction band, of layered and quasi-one-dimensional compounds, and of superconductors with A15 or C15 structure.

The analysis is carried out within the framework of the Bilbro-McMillan-Nakayama mode,[25,26] which is based on Gor'kov's idea that the electronic spectrum in compounds of the A15 type has a quasi-one-dimensional character, and which is also suitable for the description of compounds of the C15 type,[28] and on the basis of the model of an isotropic semimetal. In both cases the dielectrization is due not only to the instability of the ground state relative to electron-hole (exciton) pairing,[29] but also to hybridization of the electron and hole branches of the spectrum on account of the single-particle interband periods.[30] The reason why the paramagnetic limit is exceeded is that the existence of a dielectric gap Σ on the FS, together with a superconducting gap Δ, prevents the redistribution of the electrons among the spin subbands, thereby preserving the congruence of the FS for electrons with antiparallel spins in magnetic fields $H>H_p$. The effect of exceeding the paramagnetic limit H_{p0} is particularly large for the isotropic model, for in this case, just as in superconductors with tight binding, the BCS relation between Δ_0 and T_c does not hold, with T_c decreasing rapidly with increasing Σ,[30,31] so that the true paramagnetic limit $H_p^*\approx\Delta_0/\mu_B$ can substantially exceed $H_{p0}\approx T_c/\mu_B$.

2. MODEL HAMILTONIAN AND DYSON-GOR'KOV EQUATIONS FOR THE GREEN'S FUNCTIONS IN A MAGNETIC FIELD

We consider a multicomponent electron system whose spectrum contains several branches of elementary excitations of electron and hole type. Such a system in an external magnetic field $\mathbf{H}_0 \parallel 0Z$ without allowance for the diamagnetic effects[1)] can be described by a Hamiltonian of the type

$$\mathscr{H}=\sum_{\mathbf{p}j}\sum_{\alpha\beta}[\xi_j(\mathbf{p})\delta_{\alpha\beta}-\mu_B H_0\sigma_z^{\alpha\beta}]a_{j\alpha}^+(\mathbf{p})a_{j\beta}(\mathbf{p})$$
$$+\frac{1}{2}\sum_{\mathbf{p}\mathbf{p}'\mathbf{q}}\sum_{\alpha\beta}\sum_{ijlm}V_{ij,lm}(\mathbf{q})a_{i\alpha}^+(\mathbf{p}+\mathbf{q})a_{j\beta}^+(\mathbf{p}'-\mathbf{q})a_{m\beta}(\mathbf{p}')a_{l\alpha}(\mathbf{p}). \quad (1)$$

Here $\xi_j(\mathbf{p})$ is the energy of the j-th branch (band) of the nonrestructured electron spectrum, reckoned from the Fermi level; $\sigma_z^{\alpha\beta}$ is a Pauli matrix; $a_{j\alpha}+(\mathbf{p})$ and $a_{j\alpha}(\mathbf{p})$

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are the operators of creation and annihilation of a particle with momentum $\mathbf{p}$, energy $\xi_j(\mathbf{p})$, and spin projection $\alpha=\pm 1/2$; $V_{ij,lm}(\mathbf{q})$ are the Fourier components of the matrix elements of the electron-electron interaction.

The system of equations for the normal $G_{ij}^{\alpha\beta}(\mathbf{p},\omega_n)$ and anomalous $F_{ij}^{\alpha\beta}(\mathbf{p},\omega_n)$ Green's functions[32] is of the form

$$[(i\omega_n-\xi_i)\hat{E}+\mu_B H_0\hat{\sigma}_z]\hat{G}_{ij}+\hat{\Sigma}_{ik}\hat{G}_{kj}+\hat{\Delta}_{ik}\hat{F}_{kj}^+=\delta_{ij}\hat{E}, \tag{2}$$

$$[(i\omega_n+\xi_i)\hat{E}-\mu_B H_0\hat{\sigma}_z]\hat{F}_{ij}^++\hat{\Sigma}_{ik}^+\hat{F}_{kj}^+-\hat{\Delta}_{ik}^+\hat{G}_{kj}=0. \tag{3}$$

The self-energy parts $\hat{\Sigma}_{ij}^{\alpha\beta}$ and $\Delta_{ij}^{\alpha\beta}$ satisfy the self-consistency equations

$$\hat{\Sigma}_{ij}(\mathbf{p})=T\sum_{\omega_n}\int\frac{d\mathbf{q}}{(2\pi)^3}\{V_{ij,lm}(\mathbf{p}-\mathbf{q})\hat{G}_{lm}(\mathbf{q},\omega_n)$$

$$-\hat{E}V_{im,jl}(\mathbf{p}-\mathbf{q})\,\mathrm{Sp}\,\hat{G}_{lm}(\mathbf{q},\omega_n)\}, \tag{4}$$

$$\hat{\Delta}_{ij}(\mathbf{p})=T\sum_{\omega_n}\int\frac{d\mathbf{q}}{(2\pi)^3}V_{ij,lm}(\mathbf{p}-\mathbf{q})\hat{F}_{lm}(\mathbf{q},\omega_n). \tag{5}$$

We seek the solution of the Dyson-Gor'kov equation (2), (3) in the form

$$\hat{G}_{ij}=\hat{E}G_{ij}^s+\hat{\sigma}_z G_{ij}^t,\quad \Sigma_{ij}=\hat{E}\Sigma_{ij}^s+\hat{\sigma}_z\Sigma_{ij}^t,$$
$$\hat{F}_{ij}=\hat{I}F_{ij},\quad \hat{\Delta}_{ij}=\hat{I}\Delta_{ij},\quad (\hat{I})^2=-\hat{E}. \tag{6}$$

The presence of singlet self-energy parts Σ_{ii}^s diagonal in the band indices leads, as is well known, only to a renormalization of the chemical potential and of the effective mass of the electrons. The triplet self-energy parts Σ_{ii}^t that describe the effects of exchange (Stoner) magnetization in the self-consistent-field approximation are taken into account by replacing the external magnetic field H by the effective magnetic field $H=H_0+\Sigma_{ii}^t/\mu_B$. In addition, in the absence of instability relative to a transition into the state of an excitonic ferromagnet 33 we can put $\Sigma_{ij}^t\neq 0(i\neq j)$.

On the other hand, in the presence of degeneracy between the electron and hole branches of the spectrum, at least on a part of the FS,[25,26] on account of the different types of interaction, a nonzero singlet dielectric of order parameter $\Sigma_{ij}^s\neq 0(i\neq j)$ is produced.

On going into the superconducting state, the quasiparticle spectrum acquires, besides the dielectric gap, a superconducting gap whose width is determined by the order parameters $\Delta_{ii}\neq 0$ that are diagonal in the band indices. The off-diagonal order parameters $\Delta_{ij}(i\neq j)$ can be neglected because of the noncongruence of the FS sections in the different bands and the small probability of the interband transitions (see Ref. 30).

We consider for the sake of argument the simple model, used in Refs. 25 and 26, of an anisotropic metal whose electron spectrum consists of three branches with energies $\xi_1(\mathbf{p})$, $\xi_2(\mathbf{p})$, and $\xi_3(\mathbf{p})$ reckoned from the Fermi level. On one section of the FS the $\xi_1(\mathbf{p})$ spectrum is nondegenerate and there is no dielectric gap, while on the other section of the FS there is degeneracy of the spectrum, so that the electron and hole branches are connected by the relation $\xi_2(\mathbf{p})=-\xi_3(\mathbf{p})$ and the corresponding dielectric order parameter is $\Sigma_{23}^s\neq 0$.

In this case the matrix elements of the electron-electron interaction have the following symmetry properties:

$$V_{ij,ij}=V_{ji,ji},\quad V_{ii,jj}=V_{ij,ji}=V_{jj,ii}=V_{ji,ij},$$
$$V_{ii,ij}=V_{ii,ji}=V_{ij,ii}=V_{ji,ii},\quad i\neq j. \tag{7}$$

We introduce the notation

$$\begin{aligned}&V_1\equiv V_{11,11},\quad V_2\equiv V_{22,22}=V_{33,33},\\ &\tilde{V}\equiv V_{23,23},\quad U\equiv V_{11,22}=V_{11,33},\\ &\tilde{U}\equiv V_{22,33},\quad \tilde{W}\equiv V_{23,23}=V_{33,32}.\end{aligned} \tag{8}$$

We confine ourselves henceforth to the case of contact interaction, when the matrix elements (7) do not depend on the momentum transfer.

Substituting the solutions of the Gor'kov-Dyson equations (2), (3) into the equations (4), (5) for the order parameter and introducing

$$\Delta_1=\Delta_{11},\quad \Delta_2=\Delta_{22}=\Delta_{33},\quad \Sigma=\Sigma_{23}^s, \tag{9}$$

we obtain, taking the symmetry properties (7) and (8) into account,

$$\Delta_1=-N_1(0)V_1\Delta_1 I_1(\Delta_1)-N_2(0)U\Delta_2 I_2(\Delta_2,\Sigma), \tag{10}$$

$$\Delta_2=-{}^1/{}_2N_2(0)(V_2+\tilde{U})\Delta_2 I_2(\Delta_2,\Sigma)-N_1(0)U\Delta_1 I_1(\Delta_1), \tag{11}$$

$$\Sigma\{1-{}^1/{}_2N_2(0)(\tilde{V}-3\tilde{U})I_2(\Delta_2,\Sigma)\}=n_2\tilde{W}, \tag{12}$$

where

$$I_1(\Delta)=\int_0^{\omega_D}\frac{d\xi}{2(\xi^2+\Delta^2)^{1/2}}\left[\mathrm{th}\left(\frac{h+(\xi^2+\Delta^2)^{1/2}}{2T}\right)-\mathrm{th}\left(\frac{h-(\xi^2+\Delta^2)^{1/2}}{2T}\right)\right], \tag{13}$$

$$I_2(\Delta,\Sigma)=\int_0^{\Omega}\frac{d\xi}{2(\xi^2+\Delta^2+\Sigma^2)^{1/2}}\left[\mathrm{th}\left(\frac{h+(\xi^2+\Delta^2+\Sigma^2)^{1/2}}{2T}\right)\right.$$
$$\left.-\mathrm{th}\left(\frac{h-(\xi^2+\Delta^2+\Sigma^2)^{1/2}}{2T}\right)\right], \tag{14}$$

$N_1(0)$ and $N_2(0)$ are the respective state densities on the nondegenerate and degenerate FS sections, per spin, $h=\mu_B H$, n_2 is the concentration of the electrons (holes) in the overlapping bands, ω_D is the limiting (Debye) frequency of the phonon, and Ω is the characteristic cutoff energy of the electron-electron interaction. It coincides with ω_D in Eq. (11) and is of the order of the Fermi energy E_F or of the band width E_B in (12). The order parameters Δ_1 and Δ_2 can be chosen to be real because of the gauge invariance of (10) and (11), while Σ is real because the matrix element $\tilde{W}$ is real.

3. CRITICAL TEMPERATURE OF SUPERCONDUCTING TRANSITION AND THE PARAMAGNETIC LIMIT

We consider a superconductor with a degenerate spectrum and with a dielectric gap on the FS, and located in a magnetic field. In the case of strong mixing of the states corresponding to different branches of the electron spectrum,[25] when the matrix elements of the interaction are connected by the relation

$$V_1=V_2=U=\tilde{U}\equiv -V<0, \tag{15}$$

the system (10) and (11) reduces to a single equation for the superconducting order parameter $\Delta=\Delta_1=\Delta_2$:

$$1=V[N_1(0)I_1(\Delta)+N_2(0)I_2(\Delta,\Sigma)]. \tag{16}$$

In the absence of a magnetic field ($h=0$) the critical superconducting transition temperature T_c is determined from the equation

$$\frac{1}{V}=N_2(0)\int_0^{\omega_D}\frac{d\xi}{(\xi^2+\Sigma^2)^{1/2}}\,\mathrm{th}\,\frac{(\xi^2+\Sigma^2)^{1/2}}{2T_c}+N_1(0)\int_0^{\omega_D}\frac{d\xi}{\xi}\,\mathrm{th}\,\frac{\xi}{2T_c},\tag{17}$$

which can be solved analytically in the limiting cases of small and large Σ.

Thus, at $(\Sigma/T_c)^2 \ll 1$ it follows from (17) that (cf. Ref. 30)

$$T_c\approx T_{c0}\left[1-\frac{N_2(0)}{N(0)}\frac{7\zeta(3)}{8\pi^2}\frac{\Sigma^2}{T_{c0}^2}\right],\tag{18}$$

where $T_{c0}=(\gamma/\pi)2\omega_D\exp[-1/N(0)V]$ is the critical temperature at $\Sigma=0$; $N(0)=N_1(0)+N_2(0)$ is the total density of the electronic states on the FS, and $\zeta(x)$ is the Riemann zeta function.

In the opposite case when $(\Sigma/T_c)^2 \gg 1$ the critical temperature T_c is a solution of the transcendental equation

$$\ln\left[\left(\frac{\Delta_0}{\Sigma}\right)\left(\frac{T_{c0}}{T_c}\right)^{\nu}\right]=\left(\frac{2\pi T_c}{\Sigma}\right)^{1/2}\exp\left(-\frac{\Sigma}{T_c}\right),\tag{19}$$

where

$$\Delta_0=\pi T_{c0}/\gamma,\quad \nu=N_1(0)/N_2(0).\tag{20}$$

The limiting magnetic field at which the superconductivity is destroyed by the paramagnetic effect is determined from the condition for the existence of a solution of Eq. (16) for Δ at $h\neq 0$ and $T=0$. Depending on the relation between the quantities h, Δ, and Σ, Eq. (16) has besides the trivial nonsuperconducting solution ($\Delta=0$) three superconducting solutions with $\Delta\neq 0$ in the region of values $h<\Delta_0$; these solutions are determined at $T=0$ by the equations

$$\Delta^{\nu}(\Delta^2+\Sigma^2)^{1/2}=\Delta_0^{\nu+1},\quad h<\Delta,\tag{21}$$

$$(h+(h^2-\Delta^2)^{1/2})^{\nu}(\Delta^2+\Sigma^2)^{1/2}=\Delta_0^{\nu+1},\quad \Delta<h<(\Delta^2+\Sigma^2)^{1/2},\tag{22}$$

$$(h+(h^2-\Delta^2)^{1/2})^{\nu}(h+(h^2-\Delta^2-\Sigma^2)^{1/2})=\Delta_0^{\nu+1},\quad h>(\Delta^2+\Sigma^2)^{1/2}.\tag{23}$$

It is assumed here that Σ is constant, inasmuch as in the region of not too strong fields ($h<\Delta_0$), as follows from (12), Σ depends weakly on h at $\bar{W}\neq 0$. For arbitrary values of Σ and ν, Eqs. (21)–(23) can not be solved exactly. We consider therefore first the limiting case of total dielectrization of the FS in isotropic-semimetal model, when $\nu=0$, and then the case of partial dielectrization in the anisotropic Bilbro-McMillan-Nakayama model,[25,26] which describes well, under the condition $\Sigma \gg T_c$, the experimental situation for superconducting C15 compounds[15-18] and layered superconductors based on dichalcogenides of transition metals.[14]

A. Isotropic semimetal (complete dielectrization). In an isotropic intrinsic semimetal the degeneracy of the electron spectrum takes place on the entire FS, so that $N_1(0)=0$ and $N_2(0)\equiv N(0)$. The dielectric gap Σ in the absence of superconductivity is then defined, in accordance with (12), by the equation

$$\Sigma\left\{1-\Lambda\int_0^{\Omega}\frac{d\xi}{2(\xi^2+\Sigma^2)^{1/2}}\left[\mathrm{th}\left(\frac{h+(\xi^2+\Sigma^2)^{1/2}}{2T}\right)-\mathrm{th}\left(\frac{h-(\xi^2+\Sigma^2)^{1/2}}{2T}\right)\right]\right\}=2\rho\Omega,\tag{24}$$

where

$$\Lambda={}^1/_2N(0)(\bar{V}-3\bar{U}),\quad \rho=n_2\bar{W}/2\Omega.\tag{25}$$

It follows from (24) that because of the finite probability of the single-particle interband transitions ($\rho\neq 0$) the dielectric gap on the Fermi surface depends little on the magnetic field at $h<\Sigma$ and is different from zero at any sign of the electron-hole interaction constant Λ (see Ref. 30). Nevertheless, a phase transition to a superconducting phase (mixed SD phase) with nonzero superconducting order parameter Δ is possible in such a system if $\Sigma<\Delta_0$. The critical temperature T_c of the transition is determined at $h=0$, according to (17), by the equation[31]

$$\ln\frac{T_c}{T_{c0}}=\int_0^{\infty}d\xi\left[\frac{1}{(\xi^2+\Sigma^2)^{1/2}}\,\mathrm{th}\,\frac{(\xi^2+\Sigma^2)^{1/2}}{2T_c}-\frac{1}{\xi}\,\mathrm{th}\,\frac{\xi}{2T_c}\right].\tag{26}$$

The dependence of T_c on Σ, obtained from (26), is shown in Fig. 1. We see that $T_c\neq 0$ only in the region $\Sigma<\Delta_0$.

At $T=0$ the solutions (21) and (22) coincide in this case ($\nu=0$), and as a result we obtain in lieu of (21)–(23) two superconducting solutions

$$\Delta_1=(\Delta_0^2-\Sigma^2)^{1/2},\quad h<\Delta_0,\tag{27}$$

$$\Delta_2=[\Delta_0(2h-\Delta_0)-\Sigma^2]^{1/2},\quad {}^1/_2\Delta_0<h<\Delta_0.\tag{28}$$

The solution (27) is of the BCS type and vanishes at $\Sigma=\Delta_0$, in agreement with the result for the critical temperature. The solution (28) is a generalization of the Sarma solution,[24] which exists only in the presence of a magnetic field.

The changes of the free energy on going from the dielectric (D) to the superconducting (SD) phase are respectively for the states (27) and (28)

$$\delta F_{SD}^{(1)}=-N(0)[{}^1/_2(\Delta_0^2-\Sigma^2)+\Sigma^2\ln(\Sigma/\Delta_0)],\tag{29}$$

$$\delta F_{SD}^{(2)}=-N(0)[2h\Delta_0-h^2-{}^1/_2(\Delta_0^2-\Sigma^2)+\Sigma^2\ln(\Sigma/\Delta_0)].\tag{30}$$

From (29) and (30) it follows that the free-energy difference $\delta F_{SD}^{(1)}-\delta F_{SD}^{(2)}=-N(0)(\Delta_0-h)^2<0$, so that the solution (28) is always energywise unsuitable, just as the Sarma solution.[34]

On the other hand, in the absence of superconductivity ($\Delta=0$) at $h>\Sigma$ the dielectric (D) phase goes over into the paramagnetic (DP) phase, which is characterized by a nonzero magnetization

$$M_z=2\mu_BN(0)(h^2-\Sigma^2)^{1/2}.$$

A transition from the D into the (DP) phase is possible if the decrease of the energy on account of the ordering of the spins in the magnetic field compensates for the

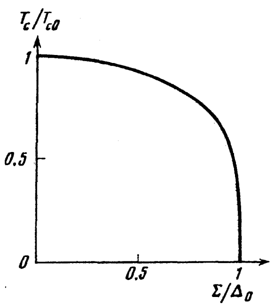

FIG. 1. Dependence of the ratio T_c/T_{c0} on the value of Σ/Δ_0 for the isotropic-semimetal model.

increase of the electron kinetic energy when they are redistributed over the spin subbands. The change of the free energy is in this case

$$\delta F_{DP}=-N(0)\left[h(h^2-\Sigma^2)^{1/2}+\Sigma^2\ln\left(\frac{\Sigma}{h+(h^2-\Sigma^2)^{1/2}}\right)\right]. \tag{31}$$

Comparing the free energies (29) and (31) for the *SD* and *DP* phases, we obtain the equation for the boundary between them:

$$\frac{1}{2}(\Delta_0^2-\Sigma^2)-h(h^2-\Sigma^2)^{1/2}+\Sigma^2\ln\left(\frac{h+(h^2-\Sigma^2)^{1/2}}{\Delta_0}\right)=0. \tag{32}$$

At the same time, the boundary of the *D* and *SD* phases is determined by the condition $\delta F_{SD}^{(1)}=0$, which is satisfied at $\Sigma=\Delta_0$.

In that phase-plane region where there is no superconductivity ($\Delta=0$) we obtain from the condition $\delta F_{DP}=0$ the boundary of the *D* and *DP* phases: $h=\Sigma$.

The phase diagram of an intrinsic semimetal in a magnetic field is shown, in the plane of the parameters Σ/Δ_0 and $\mu_B H/\Delta_0$, in Fig. 2.

We see that at $\Sigma\neq 0$ the limiting magnetic field of the *SD* phase $H_p^*>\Delta_0/\mu_B\sqrt{2}$, i.e., it always exceeds the Clogston-Chandrasekhar paramagnetic limit. On the other hand, as seen from Fig. 1, the presence of a finite dielectric gap leads to a decrease of T_c compared with T_{c0}, by virtue of which the true paramagnetic limit of the *SD* phase $H_p^*\approx\Delta_0/\mu_B$ can greatly exceed the value $H_{p0}\approx T_c/\mu_B$.

B. Anisotropic model (partial dielectrization). Assume that the electron spectrum on part of the FS is nondegenerate and there is no dielectric gap, i.e., the state density $N_1(0)\neq 0$. In this case, under the condition $\Sigma\gg\Delta$, we obtain from (21), accurate to terms $\sim(\Delta/\Sigma)^2$, a solution of the BCS type, independent of the magnetic field:

$$\Delta\approx\Sigma(\Delta_0/\Sigma)^{(\nu+1)/\nu},\quad h<\Delta, \tag{33}$$

which is valid only at $\Sigma\gg\Delta_0$. It is easy to show that the solutions that follow from (22) and (23) are generalizations of the Sarma solution and are thermodynamically unsuitable.

On the other hand, at $\Sigma\gg T_c$, we get from (19) with exponential accuracy

$$T_c\approx T_{c0}\left(\frac{\Delta_0}{\Sigma}\right)^{1/\nu}=\frac{\gamma}{\pi}\Sigma\left(\frac{\Delta_0}{\Sigma}\right)^{(\nu+1)/\nu}. \tag{34}$$

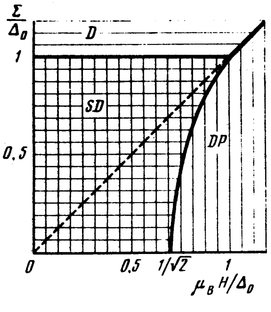

FIG. 2. Phase diagram of intrinsic semimetal in a magnetic field, in the plane of the parameters Σ/Δ_0 and $\mu_B H/\Delta_0$.

Comparing (34) with (33), we see that in this case, in contrast to the isotropic model, the BCS-theory relation between Δ and T_c is satisfied.

To find the paramagnetic limit it suffices to compare the free energies of the superconducting (*S*) and paramagnetic (*P*) phases in the region of the fields $h\ll\Sigma$, since the solution (33) for a superconducting order parameter Δ was obtained under the condition $\Sigma\gg\Delta$ and exists in fields $h<\Delta$. We note that at $h<\Sigma$ and $T=0$ a paramagnetic contribution to the free energy of the normal state ($\Delta=0$) is made only by electrons from that part of the FS where there is no dielectric gap, so that $\delta F_p=-N_1(0)h^2$. On the contrary, since the superconductivity in the case of strong mixing of the branches is due to the electrons on the entire FS, the change of the free energy following the superconducting transition is determined by the summary state density $N(0)$, and its value in the absence of a magnetic field ($h=0$) is $\delta F_s=-1/2N(0)\Delta^2$. The limiting magnetic field, determined from the condition $\delta F_p=\delta F_s$ is, when account is taken of the restriction $h<\Delta$,

$$H_p^*=\begin{cases}(\Delta/\mu_B\sqrt{2})\,[1+N_2(0)/N_1(0)]^{1/2}, & N_2(0)<N_1(0),\\ \Delta/\mu_B & N_2(0)\geqslant N_1(0).\end{cases} \tag{35}$$

It is seen that also in the case of the anisotropic model H^* always exceeds the Clogston-Chandrasekhar limit $\Delta/\mu_B\sqrt{2}$. So far we have considered the case of strong mixing of the branches, when relation (15) is satisfied. At the same time it is of interest to consider the opposite case of weak mixing of the states on the degenerate and nondegenerate parts of the FS, when the matrix element of the two-particle transitions $U\to 0$. The equations (10) and (11) are then uncoupled and take the form

$$1=-N_1(0)V_1I_1(\Delta_1), \tag{36}$$

$$1=-{}^1/_2N_2(0)(V_2+\bar{U})I_2(\Delta_2,\Sigma). \tag{37}$$

According to (36) and (37), in a model with weak mixing of the branches the partial dielectrization of the electron spectrum influence the size of the superconducting gap only on the degenerate part of the FS with state density $N(0)$. At $h=0$ we get from (36) the known BCS-theory expression for the critical temperature $T_{c1}=2\gamma\pi^{-1}\omega_D\exp\{-1/\lambda_1\}$, where $\lambda_1=-N_1(0)V_1>0$. Equation (37) linearized in Δ_2 coincides, apart from the notation, with Eq. (26) for T_c in the isotropic-semimetal model, and consequently $T_{c2}\neq 0$ only under the condition $\Sigma<\Delta_{20}\equiv 2\omega_D\exp\{-1/\lambda_2\}$, where $\lambda_2=-1/2N_2(0)(V_2+\bar{U})>0$.

The critical temperature of the superconducting transition is determined in this case by the larger of the temperatures T_{c1} and T_{c2}, although in principles two successive superconducting transitions can be observed on the temperature dependences of the heat capacity and of the magnetic susceptibility, which are sensitive to changes of the state density on the FS (see Ref. 35).

If $\lambda_2>\lambda_1$, i.e., $\Delta_{20}>\Delta_{10}\equiv\pi T_{c1}/\gamma$, then independently of the ratio of T_{c1} and T_{c2} the Clogston-Chandrasekhar paramagnetic limit is exceeded. Indeed, at small λ_1, when the critical temperature $T_{c2}>T_{c1}$ despite the presence of the dielectric gap $\Sigma\neq 0$, the paramagnetic limit $H_p^*\approx\Delta_{20}/\mu_B$ of an anisotropic metal, just as in the case of an isotropic semimetal,[31] can greatly exceed the value $H_{p0} \cong 18.4T_{c2}$ [kG]. At $T_{c1} > T_{c2}$ (but $\Delta_{10} < \Delta_{20}$) the paramagnetic limit H_p^* is also determined by the value of Δ_{20} and exceeds $H_{p0} = 18.4T_{c1}$ [kG]. We note that in this case the critical temperature $T_c \equiv T_{c1}$ does not depend on the value of the dielectric gap Σ and can be quite high. Finally, if $\lambda_1 > \lambda_2$, then $\Delta_{10} > \Delta_{20}$ and $T_{c1} > T_{c2}$ so that the paramagnetic limit is not exceeded (at least in the weak-binding approximation).

4. DISCUSSION OF RESULTS

As already noted, the Bilbro-McMillan-Nakayama model describes well compounds with C15 structure, which include HfV_2 and ZrV_2. A characteristic feature of of these compounds is the structural phase transition in the temperature region $T \approx (120-150)$K, accompanied by partial dielectrization of the electron spectrum.[16-18] According to the measurements[36] of the specific heat and of the magnetic susceptibility, the ratio of the state densities on the degenerate and nondegenerate parts of the FS is $N_2(0)/N_1(0) \approx 0.78$ for HfV_2 and $N_2(0)/N_1(0) \approx 0.92$ for ZrV_2. The critical temperatures of the superconducting transition for HfV_2 and ZrV_2 are respectively equal to $T_c = 9.0$ and $T_c = 8.9$ K according to the data of Refs. 16 and 36 and $T_c = 9.6$ and $T_c = 8.8$ K according to the data of Ref. 1. Unfortunately there are no reliable measurements of the upper critical field $H_{c2}(0)$ for these compounds. In Ref. 1, however, are given the measured values of $H_{c2}(T)$ for the intermediate compositions $Hf_{0,5}Zr_{0,5}V_2$ and $Hf_{0,4}Zr_{0,6}V_2$ with $T_c = (10.1-10.2)$, according to which $H_{c2}(T)$ at $T = 4.2$ are respectively 230 and 208 kG, and extrapolation to $T = 0$ for the second composition yields $H_{c2}(0) = 254$ kG. If we assume that the shape of the FS and the state densities of the isoelectronic compounds with intermediate composition $Hf_xZr_{1-x}V_2$ are such that the ratio $N_2(0)/N_1(0)$ lies in the interval between its values for the extreme compositions HfV_2 and ZrV_2 (Ref. 36), then we obtain from (35) the following estimate for the paramagnetic limit: $H_p^* \approx (250-260)$ kG, in good agreement with the experimental data[1] for $H_{c2}(0)$.

At the same time, the two- or threefold excess above the paramagnetic limit observed in some superconductors (e.g., in Chevrel phases[2] and in layered dichalcogenides of transition metals[4]) can be explained on the basis of the model considered above, of an isotropic metal with weak mixing of the states.

Thus, partial or total dielectrization of the electron spectrum as a result of structural instability can explain the excess above the paramagnetic limit $H_{p0} = 18.4\, T_c$ [kG] for a large number of superconducting compounds[1-6] without resorting to a special mechanism for each concrete material. An additional argument favoring this point of view, first advanced in Ref. 31 and considered in detail in the present paper, is the fact that the coexistence of supercondictivity and weak impurity ferromagnetism with Curie temperature $T_k \approx T_c$ is most frequently observed in compounds with C15 structure (Laves phases).[37] In fact, as shown above, the quantity h contains not only an external field H_0, but also an exchange field $\tilde{H} = \Sigma_t/\mu_B$, connected with the orientation of the spins in the bands. Therefore the increase of the paramagnetic limit increases simultaneously also the limiting value of the exchange field of the magnetically ordered impurities, and it is this field which destroys the superconductivity.

[1)]In "hard" type-II superconductors the limitation on the upper critical field $H_{c2}(0)$ is due to paramagnetic effects.[2]

1. K. Inoue and K. Tachikawa, Appl. Phys. Lett. **29**, 386 (1976).
2. S. Fischer, Appl. Phys. **16**, 1 (1978).
3. S. Alterovitz and J. A. Woollam, Solid State Commun. **25**, 141 (1978).
4. L. N. Bulaevskiĭ, Usp. Fiz. Nauk **116**, 449 (1975); **120**, 259 (1978) [Sov. Phys. Usp. **18**, 514 (1975); **19**, 836 (1978)].
5. J. A. Woollam and R. B. Somoano, Phys. Rev. **B13**, 3843 (1976).
6. L. J. Azevedo, W. G. Clark, G. Deutscher, R. Greene, G. B. Street, and L. J. Suter, Solid State Commun. **19**, 197 (1976).
7. L. N. Bulaevskiĭ, Zh. Eksp. Teor. Fiz. **65**, 1278 (1973) [Sov. Phys. JETP **38**, 634 (1974)].
8. R. A. Klemm, A. Luther, and M. Beasley, Phys. Rev. **B12**, 877 (1975).
9. L. N. Bulaevskiĭ, A. A. Guseĭnov, and A. I. Rusinov, Zh. Eksp. Teor. Fiz. **71**, 2356 (1976) [Sov. Phys. JETP **44**, 1243 (1976)].
10. V. Jaccarino and M. Peter, Phys. Rev. Lett. **9**, 290 (1962).
11. K. B. Efetov and A. I. Larkin, Zh. Eksp. Teor. Fiz. **68**, 155 (1975) [Sov. Phys. JETP **41**, 76 (1975)].
12. K. B. Efetov, Zh. Eksp. Teor. Fiz. **73**, 1944 (1977) [Sov. Phys. JETP **46**, 1020 (1977)].
13. S. Maekawa and M. Tachiki, Phys. Rev. **B18**, 4688 (1978).
14. B. T. Geĭlikman and V. Z. Kresin, Fiz. Tverd. Tela (Leningrad) **7**, 3294 (1965) [Sov. Phys. Solid State **7**, 2659 (1966)].
15. A. C. Lawson and W. H. Zachariasen, Phys. Lett. **A38**, 1 (1972). A. C. Lawson, Phys. Rev. **B17**, 1136 (1978).
16. V. M. Pan, I. E. Bulakh, A. L. Kasatkin, and A. D. Shevchenko, Pis'ma Zh. Eksp. Teor. Fiz. **27**, 629 (1978) [JETP Lett. **27**, 594 (1978)]; Fiz. Tverd. Tela (Leningrad) **20**, 2487 (1978) [Sov. Phys. Solid State **20**, 1437 (1978)].
17. J. W. Jafstrom, G. S. Knapp, and A. T. Aldred, Phys. Rev. **B17**, 2892 (1978).
18. M. Levinson, C. Zahradnic, R. Bergh, M. I. McVicar, and J. Bostock, Phys. Rev. Lett. **41**, 899 (1978).
19. A. C. Lawson, Mater. Res. Bull. **7**, 733 (1972).
20. D. C. Johnston, R. M. Shelton, and J. J. Bugai, Solid State Commun. **21**, 949 (1977).
21. R. Flükiger, A. Junod, R. Spitzli, A. T. Treyvaud, A. Paoli, H. Devantay, and J. Muller, Solid State Commun. **23**, 669 (1977).
22. V. V. Walatka, M. M. Labes, and J. H. Perlstein, Phys. Rev. Lett. **31**, 1139 (1973).
23. A. N. Bloch, D. O. Cowan, K. Bechgaard, R. E. Pyle, R. H. Banks, and T. O. Poehler, Phys. Rev. Lett. **34**, 1561 (1975).
24. C. Weyl, E. M. Engler, K. Bechgaard, G. Jehanno, and S. Etemad, Solid State Commun. **19**, 925 (1976).
25. G. Bilbro and W. L. McMillan, Phys. Rev. **B13**, 1887 (1976).
26. I. Nakayama, J. Phys. Soc. Jpn. **43**, 1533 (1977).
27. L. P. Gor'kov, Zh. Eksp. Teor. Fiz. **65**, 1658 (1973) [Sov. Phys. JETP **38**, 830 (1974)].
28. Yu. A. Izyumov, V. E. Naish, and V. N. Syromyatnikov, Fiz. Met. Metalloved. **39**, 455 (1975).
29. L. V. Keldysh and Yu. V. Kopaev, Fiz. Tverd. Tela (Leningrad) **6**, 2791 (1964) [Sov. Phys. Solid State **6**, 2219 (1965)].

[30]A. M. Gabovich, E. A. Pashitskiĭ, and A. S. Shpigel', Fiz. Tverd. Tela (Leningrad) **18**, 3279 (1976) [Sov. Phys. Solid State **18**, 1911 (1976)].
[31]A. M. Gabovich, E. A. Pashitskiĭ, and A. S. Shpigel', Pis'ma Zh. Eksp. Teor. Fiz. **28**, 302 (1978) [JETP Lett. **28**, 277 (1978)].
[32]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].
[33]B. A. Volkov, Yu. V. Kopaev, and A. I. Rusinov, Zh. Eksp. Teor. Fiz. **68**, 1899 (1975) [Sov. Phys. JETP **41**, 952 (1975)].
[34]G. Sarma, J. Phys. Chem. Solids **24**, 1029 (1963).
[35]M. Dayan, A. M. Goldman, C.-C. Huang, M. C. Chiang, and and L. E. Toth, Phys. Rev. Lett. **42**, 335 (1979).
[36]V. M. Pan, I. E. Bulakh, A. L. Kasatkin, and A. D. Shevchenko, J. Less-Common Met. **62**, 157 (1978).
[37]S. Roth, Appl. Phys. **15**, 1 (1978).

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Investigation of the effect of surface scattering of electrons on the radio-frequency size effect in tungsten

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The radio-frequency size effect (RSE) and the magnetoresistance are experimentally investigated in a magnetic field parallel to the surface of tungsten single-crystal plates in the {110} plane, placed in a high vacuum and having different surface states: a) with adsorbed residual-gas film and b) cleaned by heating to high temperature. It is observed the surface cleaning decreases the amplitudes of the RSE lines but leaves their widths and shapes unchanged. The weakening of the RSE does not depend substantially on the positions of the orbits on the electron jack and on the hole octahedron, manifests itself weakly for the spheroid lines, and correlates with the variation of the magnetoresistance. The connection of the amplitude and width of the RSE lines with the specularity coefficient are analyzed in light of the existing theories. It is shown that the observed sensitivity of the RSE to the surface state is well described by the variation of the specularity coefficient of the grazing electrons. The changes of *p* determined from the RSE measurement agree qualitatively with the corresponding values determined by measuring the magnetoresistance.

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1. INTERACTION

It is well known that the radio-frequency size effect (RSE) in a magnetic field **H** parallel to the surface of a plane-parallel metallic plate of thickness d is due to two effects: the cutoff of the effective orbits (CEO) and the anomalous penetration (AP).[1] The theory of the CEO in a plate in the limiting cases of diffuse and specular scattering was developed by Kaner *et al.* in Refs. 2 and 3, respectively. The gist of the conclusions of the theory reduces to the following. At H_0 (where $H_0 = 2\hbar kc/ed$ is the cutoff field, $2\hbar k$ is the diameter of the electron orbit, e is the charge, and c is the speed of light) the electron trajectories cannot be fitted in the plate, so that in a metal with a diffuse boundary the extremal-section electrons which pass through the skin layer, become scattered by the opposite surface of the plate and lose the energy acquired from the wave. In a metal with a specular boundary, the colliding electrons return repeatedly to the skin layer at $H<H_0$, just as the volume electrons at $H>H_0$. In addition, in this case the skin layer is formed mainly by the surface electrons that glance over the surface along trajectories with centers outside the metal. The shunting of the contribution of the volume electrons into the high-frequency conductivity by the surface electrons, just as the conservation of the number of electrons participating in the formation of the skin layer at $H<H_0$, make the attenuation of the singularity of the impedance at specular reflection stronger than in the diffuse case.

The theory of the AP in a semi-infinite metal, in the limiting cases of diffuse ($|\gamma|\ll 1-p$) and specular [$|\gamma|(\delta_0/R)^{1/2}\gg 1-p$] scatterings, and also at intermediate values of the specularity coefficient p

$$|\gamma|(\delta_0/R)^{1/2}\ll 1-p\ll|\gamma|\ll 1 \tag{1}$$

was developed in Refs. 1–6. Here $\gamma=(\nu-i\omega)/\Omega$, δ_0 is the skin-layer depth, Ω and ω are the cyclotron and electromagnetic frequencies, respectively, ν is the collision frequency, and R is the radius of the electron trajectory. In AP, the electrons form equidistant current sheets of thickness

$$\delta_\gamma=(4c^2R\Omega\gamma/3\omega\omega_0^2)^{1/3} \tag{2}$$

(ω_0 is the plasma frequency of the metal) at a distance

