Dirac points of electron energy spectrum, band-contact lines, and electron topological transitions of $3\frac{1}{2}$ kind in three-dimensional metals

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In many three-dimensional metals with inversion symmetry and a weak spin-orbit interaction, Dirac points of the electron energy spectrum form band-contact lines in the Brillouin zones of these crystals, and electron topological transitions of $3\frac{1}{2}$ kind are due to certain points on these lines. We theoretically study these transitions in detail and point out that they can be detected with magnetic susceptibility which exhibits a giant diamagnetic anomaly at the $3\frac{1}{2}$-order transitions.

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I. INTRODUCTION

The Dirac points of electron energy spectra specify many unusual properties of graphene [1,2], of topological insulators [3–5], and of Weyl semimetals [6,7]. In this paper we call attention to the fact that in the "usual" three-dimensional (3D) metals the Dirac points can be located along band-contact lines in the Brillouin zones of the metals, the energies of the points can fill a whole interval in the energy axis [8], and these Dirac points lead to specific electron topological transitions in the 3D metals. At these transitions topology of the Fermi surface (FS) in the metals changes, but this change differs from the FS transformation at the well-known topological transitions of $2\frac{1}{2}$ kind, which were first considered by Lifshits [9]. At the topological transitions of $2\frac{1}{2}$ kind a new void of the FS appears (disappears), or a neck on the FS forms (disrupts). These transitions occur near critical points $\mathbf{p}_c$ in the Brillouin zone at which the electron energy ε has an extremum or a saddle point in its dependence on the quasimomentum $\mathbf{p}$. The small vicinities of these points give a singular van Hove contribution [10] $\delta\nu(\varepsilon_F)$ to the electron density of states $\nu(\varepsilon_F)$, $\delta\nu \propto (\varepsilon_F - \varepsilon_c)^{1/2}$, where ε_F is the Fermi energy of the metal and $\varepsilon_c = \varepsilon(\mathbf{p}_c)$ is the critical energy. In the Ω potential the appropriate singular contribution has the form $\delta\Omega(\varepsilon_F) \propto (\varepsilon_F - \varepsilon_c)^{5/2}$, and by analogy with the second-order phase transitions, the topological transitions were named the $2\frac{1}{2}$-order transitions, although they are not due to a change in any symmetry. The Lifshits topological transitions and their manifestations in various physical phenomena were studied theoretically and experimentally in many papers; see the reviews [11,12], the recent papers [13,14], and references therein. In this paper we show that the topological transitions associated with the Dirac points are widespread in metals no less than the $2\frac{1}{2}$-order transitions of Lifshits. The transitions discussed here occur at the points on the band-contact lines at which the energy of two touching bands reaches its maximum or minimum on these lines. These transitions are $3\frac{1}{2}$ kind according to the classification of Ref. [9], and we explain how these transitions can be detected in experiments.

II. BAND-CONTACT LINES

It is common knowledge that the contact of the electron energy bands in a metal can occur at symmetry points and along the symmetry axis of its Brillouin zone. Besides, as was shown by Herring [15], there are *lines of an accidental contact* between two bands in crystals. The term accidental means that the degeneracy of the electron states is not caused by their symmetry. Such band-contact lines along which the spectrum of the two bands has the Dirac form are widespread in metals with inversion symmetry and with a weak spin-orbit interaction. This follows from one of Herring's results [15]: If there is a point of an intersection of two energy bands in an axis of symmetry of the Brillouin zone, a band-contact line perpendicular to the axis has to pass through this point. An intersection of the bands at points in the axes frequently occurs even in simple metals [16]. The literature data show that the lines of the accidental contact exist, for example, in Be, Mg, Zn, Cd, Al, graphite, and many other metals. The result of Herring can be understood from the following simple considerations [17]: Let the two electron bands marked by indexes 1 and 2 be degenerate at a quasimomentum $\mathbf{p}_0$ and hence have the same energy ε_0 at this point. The $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian $\hat{H}$ for these bands in the vicinity of $\mathbf{p}_0$ has the form

$$\hat{H} = \begin{pmatrix} E_{11} & E_{12} \\ E_{12} & E_{22} \end{pmatrix}, \tag{1}$$

where $E_{12}=\mathbf{v}_{12}\cdot(\mathbf{p}-\mathbf{p}_0)$, $E_{11}=\varepsilon_0+\mathbf{v}_{11}\cdot(\mathbf{p}-\mathbf{p}_0)$, $E_{22}=\varepsilon_0+\mathbf{v}_{22}\cdot(\mathbf{p}-\mathbf{p}_0)$, and $\mathbf{v}_{ij}$ are the matrix elements of the velocity operator for the electron states 1 and 2 at point $\mathbf{p}_0$. Note that $\mathbf{v}_{12}$ and E_{12} are real quantities for metals with inversion symmetry and with negligible spin-orbit interaction. The diagonalization of the Hamiltonian (1) gives the dispersion relation for the two bands in the vicinity of point $\mathbf{p}_0$,

$$\varepsilon_{1,2}(\mathbf{p}) = \varepsilon_0 + \mathbf{v}_+\cdot(\mathbf{p}-\mathbf{p}_0) \pm \{[\mathbf{v}_-\cdot(\mathbf{p}-\mathbf{p}_0)]^2 + [\mathbf{v}_{12}\cdot(\mathbf{p}-\mathbf{p}_0)]^2\}^{1/2}, \tag{2}$$

where $\mathbf{v}_+ \equiv (\mathbf{v}_{11}+\mathbf{v}_{22})/2$, $\mathbf{v}_- \equiv (\mathbf{v}_{11}-\mathbf{v}_{22})/2$ [18]. It follows from Eq. (2) that the spectrum has the Dirac form in the plane passing through vectors $\mathbf{v}_-$ and $\mathbf{v}_{12}$, and the degeneracy of bands 1 and 2 is not lifted along the straight line passing through point $\mathbf{p}_0$ in the direction of the vector $\mathbf{z} = [\mathbf{v}_- \times \mathbf{v}_{12}]$, which is perpendicular to the plane. In other words, existence of the band-degeneracy point leads to the existence of the band-contact line passing through this point. Of course, this degeneracy line exists not only near $\mathbf{p}_0$. If one takes into account terms of higher order in $\mathbf{p}-\mathbf{p}_0$ in the expansions of E_{ij}, the band-contact line will be determined by the two equations: $E_{11}(\mathbf{p}) - E_{22}(\mathbf{p}) = 0$, $E_{12}(\mathbf{p}) = 0$. Such band-contact

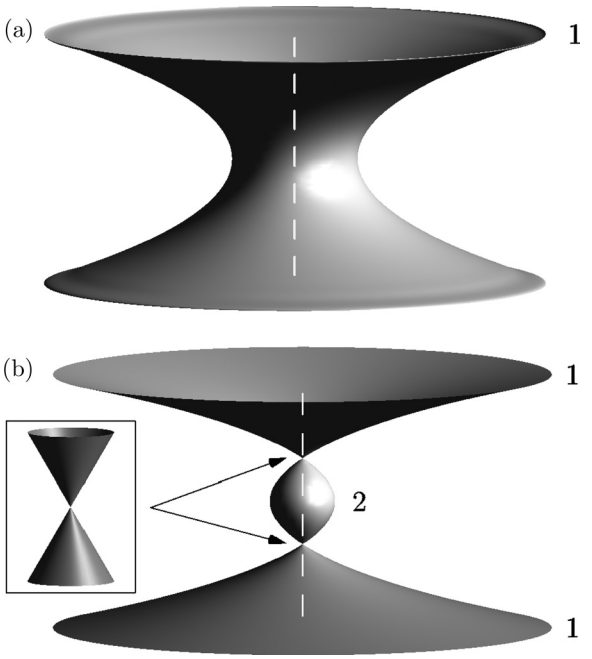

FIG. 1. The Fermi surfaces near $\varepsilon_c = \varepsilon_{\min}$ at $\tilde{a}^2 < 1$ (here $\tilde{a} = 0$): (a) $\varepsilon_F < \varepsilon_{\min}$ and (b) $\varepsilon_F > \varepsilon_{\min}$. The band-contact line is shown by the dashed line. If $\varepsilon_c - \varepsilon_{\min}$ increases, the two conical points in panel (b) become widely separated. The inset shows the FS near one of these points when $\varepsilon_{\min} < \varepsilon_F < \varepsilon_{\max}$, and ε_F is far away from these critical energies.

lines are either closed curves in the Brillouin zone or end on the surface of this zone. In both cases the energy ε_0 of the two touching bands in the degeneracy line is a periodic function of $\mathbf{p}_0$ running this line, and ε_0 changes between its minimum $\varepsilon_{\min}$ and maximum $\varepsilon_{\max}$ values. In experiments, the band-contact lines in metals can be, in principle, detected via the phase analysis of the de Haas–van Alphen (or Shubnikikov–de Haas) oscillations since the phase of these oscillations is determined by the number of the band-contact lines penetrating the appropriate cross section of the Fermi surface [19–21].

Let the Fermi level ε_F of the metal lie in the interval: $\varepsilon_{\min} < \varepsilon_F < \varepsilon_{\max}$. Then, the Fermi surface $\varepsilon_{1,2}(\mathbf{p}) = \varepsilon_F$ of this metal in the vicinity of point $\mathbf{p}_0$ defined by [22] $\varepsilon_0(\mathbf{p}_0) = \varepsilon_F$ consists of two cones with the common vertex $\mathbf{p}_0$ and the same vertex angle penetrated by the band-contact line, see the inset in Fig. 1. One of the cones corresponds to band 1, and the second cone corresponds to band 2. In other words, the Fermi surface has a self-intersecting shape [17]. At $\varepsilon_F = \varepsilon_{\min}$ this self-intersecting FS appears, and at $\varepsilon_F = \varepsilon_{\max}$ it disappears, i.e., at these critical energies the electron topological transitions occur, Figs. 1 and 2. These transitions were named the appearance (disappearance) of the self-intersecting FSs [17].

Consider now the spectrum of the two bands near the critical point $\mathbf{p}_0$ at which $\varepsilon_0(\mathbf{p}_0) = \varepsilon_c$ where $\varepsilon_c = \varepsilon_{\min}$ or $\varepsilon_{\max}$. If $\mathbf{p}$ is measured from this $\mathbf{p}_0$, then we arrive at

$$\varepsilon_{1,2}(\mathbf{p}) = \varepsilon_c + B_+ p_\parallel^2 + \mathbf{v}_+^\perp \cdot \mathbf{p}_\perp \pm [(B_- p_\parallel^2 + \mathbf{v}_- \cdot \mathbf{p}_\perp)^2 + (B_{12} p_\parallel^2 + \mathbf{v}_{12} \cdot \mathbf{p}_\perp)^2]^{1/2}, \quad (3)$$

where $p_\parallel$ is the component of $\mathbf{p}$ parallel to vector $\mathbf{z}$, i.e., to the band-contact line at point $\mathbf{p}_0$, whereas $p_\perp$ is the component

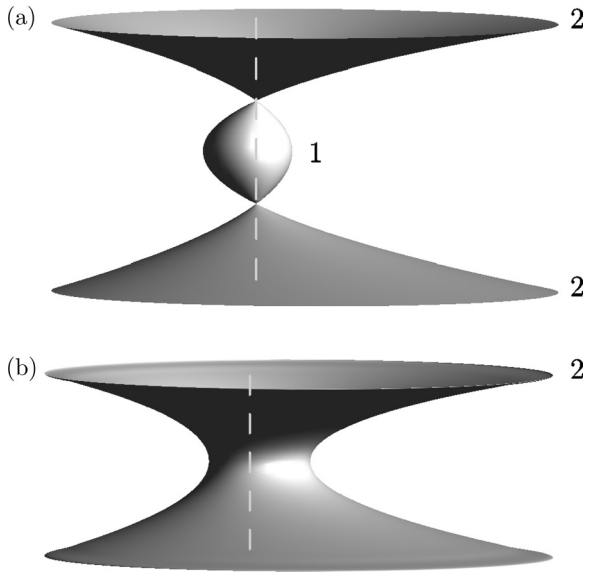

FIG. 2. The Fermi surfaces near $\varepsilon_c = \varepsilon_{\max}$ at $0 < \tilde{a}^2 < 1$: (a) $\varepsilon_F < \varepsilon_{\max}$ and (b) $\varepsilon_F > \varepsilon_{\max}$. The band-contact line is shown by the dashed line.

perpendicular to $\mathbf{z}$. Equation (3) takes into account that $\mathbf{v}_+^\parallel = 0$ at the point where ε_0 reaches its extremum, and so we have included terms proportional to $p_\parallel^2$ in the elements E_{ij} of Hamiltonian (1) (the coefficients B_+, B_-, and B_{12} are some constants; B_-, B_{12} are different from zero if the band-contact line is not a straight line, i.e, if it is not a symmetry axis of the crystal). Expression (3) is the most general form of the electron spectrum near the critical energy ε_c. To analyze this spectrum, let us set the coordinate axis z along vector $\mathbf{z}$, and hence the x-y plane coincides with the plane of vectors $\mathbf{v}_-$ and $\mathbf{v}_{12}$. Without loss of generality, we may also assume that axes p_x and p_y are chosen so that the quadratic form $(\mathbf{v}_- \cdot \mathbf{p}_\perp)^2 + (\mathbf{v}_{12} \cdot \mathbf{p}_\perp)^2$ under the root sign in Eq. (3) is diagonal and hence takes the form $b_{xx} p_x^2 + b_{yy} p_y^2$ where

$$b_{xx} = (v_-)_x^2 + (v_{12})_x^2, \quad b_{yy} = (v_-)_y^2 + (v_{12})_y^2.$$

Besides, at a fixed p_z we will measure p_x and p_y from the band-contact line, i.e., from the point $\mathbf{p}_\perp(p_z)$ defined by the equations: $\mathbf{v}_{12} \cdot \mathbf{p}_\perp + B_{12} p_z^2 = 0$, $\mathbf{v}_- \cdot \mathbf{p}_\perp + B_- p_z^2 = 0$. In this coordinate system the band-contact line is straight $p_x = p_y = 0$, and Eq. (3) reduces to the formula,

$$\varepsilon_{1,2}(\mathbf{p}) = \varepsilon_c + B p_z^2 + \mathbf{v}_+^\perp \cdot \mathbf{p}_\perp \pm \left[b_{xx} p_x^2 + b_{yy} p_y^2\right]^{1/2}, \quad (4)$$

where

$$B = \det \begin{pmatrix} B_+ & B_- & B_{12} \\ (v_+)_x & (v_-)_x & (v_{12})_x \\ (v_+)_y & (v_-)_y & (v_{12})_y \end{pmatrix} \times \left[\det \begin{pmatrix} (v_-)_x & (v_{12})_x \\ (v_-)_y & (v_{12})_y \end{pmatrix}\right]^{-1}.$$

It is important to emphasize that the spectrum (4), in fact, depends only on two essential parameters. Indeed, changing the variables p_x, p_y, and p_z as follows: $\tilde{p}_x = \sqrt{b_{xx}} p_x$, $\tilde{p}_y = \sqrt{b_{yy}} p_y$, $\tilde{p}_z = \sqrt{|B|} p_z$, and rotating the axes $\tilde{p}_x$, $\tilde{p}_y$

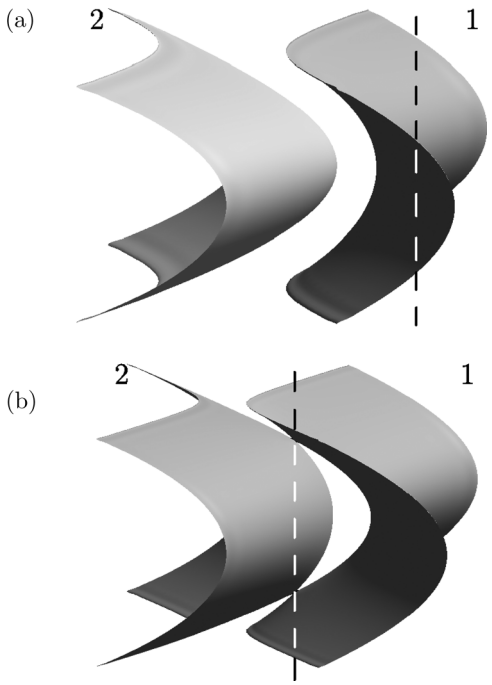

FIG. 3. The Fermi surfaces near $\varepsilon_c = \varepsilon_{\min}$ at $\tilde{a}^2 > 1$: (a) $\varepsilon_F < \varepsilon_{\min}$ and (b) $\varepsilon_F > \varepsilon_{\min}$. The band-contact line is shown by the dashed line.

through some angle, one can reduce Eq. (4) to the formula,

$$\varepsilon_{1,2}(\tilde{\mathbf{p}}) = \varepsilon_c + \mathrm{sgn}(B)\tilde{p}_z^2 + \tilde{a}\,\tilde{p}_x \pm \left[\tilde{p}_x^2 + \tilde{p}_y^2\right]^{1/2}, \quad (5)$$

where $\mathrm{sgn}(x) = \pm 1$ for $x > 0$ and $x < 0$, respectively, and

$$\tilde{a}^2 \equiv \frac{(v_+)_x^2}{b_{xx}} + \frac{(v_+)_y^2}{b_{yy}}. \quad (6)$$

Thus, the spectrum is substantially determined by a value of $\tilde{a}$ which characterizes the shape of the FS (see Figs. 1–3) and by a sign of B which specifies if the self-intersecting surfaces appear or disappear at $\varepsilon = \varepsilon_c$. The electron spectrum near any critical point of interest can be reduced to expression (5).

If a weak spin-orbit interaction is taken into account, inspection of a narrow "tube" in the place of the band-contact line becomes more appropriate in analyzing the electron energy spectra. Inside this tube the two bands closely approach each other without their touching. Hence the intersection of the appropriate Fermi surfaces, strictly speaking, does not occur (there is a small space gap between them). However, as our analysis shows, this fact has no essential effect on the results presented below, and so we, as a rule, neglect the spin-orbit interaction here. For reference, we note that with the spin-orbit interaction, the spectrum (5) transforms into

$$\varepsilon_{1,2}(\tilde{\mathbf{p}}) = \varepsilon_c + \mathrm{sgn}(B)\tilde{p}_z^2 + \tilde{a}\,\tilde{p}_x \pm \left[\Delta^2 + \tilde{p}_x^2 + \tilde{p}_y^2\right]^{1/2}, \quad (7)$$

where Δ is the energy gap between the bands at $\tilde{\mathbf{p}} = 0$. Interestingly, at $\tilde{a} \neq 0$ a minimum of the upper band and a maximum of the lower band in $\tilde{\mathbf{p}}_\perp$ occur at different values of $\tilde{\mathbf{p}}_\perp$, and the spectrum (7) is characterized by the indirect energy gap $2\Delta_{\min} = 2\Delta(1 - \tilde{a}^2)^{1/2}$. At $\tilde{a}^2 > 1$ the indirect gap is zero.

III. ELECTRON TOPOLOGICAL TRANSITIONS OF $3\frac{1}{2}$ KIND

Near $\varepsilon_F = \varepsilon_c$ the density of the electron states $\nu(\varepsilon_F)$ calculated per unit volume of the crystal is the sum of its regular part $\nu_{\mathrm{reg}}(\varepsilon_F)$ and of its singular part $\delta\nu(\varepsilon_F)$. The latter is due to the electron topological transitions mentioned above and differs from zero when $\Delta\varepsilon_F \equiv (\varepsilon_F - \varepsilon_c)\mathrm{sgn}(B) > 0$. This singular $\delta\nu(\varepsilon_F)$ exists only if $\tilde{a}^2 < 1$,

$$\delta\nu(\varepsilon_F) = \frac{4(\Delta\varepsilon_F)^{3/2}}{3\pi^2\hbar^3|B|^{1/2}(1-\tilde{a}^2)^{3/2}(b_{xx}b_{yy})^{1/2}}, \quad (8)$$

where we have taken into account the double degeneracy of the electron states in spin. At $\tilde{a} = 0$ formula (8) reproduces the density of the electron states near a critical energy in wurtzite-type crystals [17,23]. If $\tilde{a}^2 > 1$, the singular term is absent. Note that the singularity in the density of the electron states $\delta\nu \propto (\varepsilon_F - \varepsilon_c)^{3/2}$ is weaker than the singularity $\delta\nu \propto (\varepsilon_F - \varepsilon_c)^{1/2}$ at the well-known topological transitions of $2\frac{1}{2}$ kind [9,11,12,17] when a Fermi-surface void appears (disappears) or a neck of the Fermi-surface forms (disrupts). It also follows from formula (8) that the singular contribution to the Ω potential now has the form $\delta\Omega(\varepsilon_F) \propto (\varepsilon_F - \varepsilon_c)^{7/2}$, and the topological transitions considered here are the $3\frac{1}{2}$-order transitions according to the classification of Lifshits [9,17].

It is known [24] that the topological properties of any closed surface are completely determined by the number of its components (its disconnected parts) and by the number of handles for each of the components. How can the transitions consisting in appearing (disappearing) of the self-intersecting Fermi surfaces be understood from this point of view? (Recall that, in reality, there is a small gap between the touching FSs if one takes into account a weak spin-orbit interaction, and the intersection of the surfaces, strictly speaking, does not occur.) It is clear from Fig. 1 that at $\tilde{a} < 1$ the appearance of the self-intersecting FS is equivalent to the disappearance of the handle that exists in the FS of the first band at $\varepsilon_F < \varepsilon_{\min}$ and to the simultaneous appearance of the ovaloid of the second band. The transformation of the FS for the first band can also be interpreted as the disruption of the Fermi-surface neck, and the choice of the interpretation depends on the shape of this FS far away from the critical point. In Fig. 2 we show the disappearance of the self-intersecting FS in the vicinity of $\varepsilon_{\max}$ at $\tilde{a} < 1$. This transition is equivalent to the disappearance of the void of the first band and to the formation of the neck on the FS of the second band (or to the appearance of the handle in another interpretation). For these two combined transitions at $\varepsilon_{\min}$ and $\varepsilon_{\max}$, the changes in the Fermi-surface components or their handles are evident. On the other hand, at $\tilde{a} > 1$ the appearance of the self-intersecting FS does not change the number of its components and handles, Fig. 3. In other words, there is no topological transition at $\tilde{a} > 1$, and it is for this reason that the density of the electron states does not exhibit any singularity in this case. In this context, it would be more proper to name the topological transitions discussed here the combined electron topological transitions rather than the appearance (disappearance) of the self-intersecting Fermi surfaces.

At the combined topological transitions of the $3\frac{1}{2}$ kind the singularities of the physical quantities that are proportional to the density of the electron states ν or its derivative $d\nu/d\varepsilon_F$ are weaker than the singularities at the topological transitions of the $2\frac{1}{2}$ kind. This makes detection of the $3\frac{1}{2}$-order transitions difficult with measurements of these quantities. However, these transitions can be detected with magnetic susceptibility since its orbital part generally is not determined by the density of the electron states, and at the $3\frac{1}{2}$-order transitions the component χ_{zz} of the magnetic-susceptibility tensor turns out to exhibit a giant diamagnetic anomaly [25]. At low temperatures T, $T \ll \Delta\varepsilon_F$, and weak magnetic fields H, $H \ll H_T \equiv T^2c/[e\hbar(b_{xx}b_{yy})^{1/2}(1-\tilde{a}^2)^{3/2}]$, one has [25]

$$\chi^0_{zz}(\varepsilon_F) = -\frac{e^2}{6\pi^2c^2\hbar}\left(\frac{b_{xx}b_{yy}}{|B|}\right)^{1/2}\frac{(1-\tilde{a}^2)^{3/2}}{(\Delta\varepsilon_F)^{1/2}}. \qquad (9)$$

Thus, the anomaly is the large peak in the ε_F dependence of $|\chi^0_{zz}|$. Interestingly, the singularity in the susceptibility $\chi^0_{zz}(\varepsilon_F) \propto (\Delta\varepsilon_F)^{-1/2}$ is the same as the singularity in the thermoelectric power at the $2\frac{1}{2}$-order transitions [11]. The divergence of expression (9) for $\Delta\varepsilon_F \to 0$ should be cut off at $\Delta\varepsilon_F \sim T$, and this cutoff determines the magnitude of the diamagnetic peak in the weak magnetic fields.

In the case of $H > H_T$ the magnetic susceptibility near the points of the $3\frac{1}{2}$-order transitions were theoretically studied in detail in Ref. [26] using the exact expression for the electron Landau levels in the vicinity of these points at the magnetic field $\mathbf{H} \parallel \mathbf{z}$,

$$\varepsilon_{1,2}(l,\tilde{p}_z) = \varepsilon_c + \mathrm{sgn}(B)\tilde{p}_z^2 \pm \left[\frac{eH\alpha}{c\hbar}l + \Delta^2_{\min}\right]^{1/2}, \qquad (10)$$

where $\alpha = 2(b_{xx}b_{yy})^{1/2}(1-\tilde{a}^2)^{3/2}$, $\tilde{a}^2 < 1$, l is a non-negative integer ($l = 0,1,\ldots$), and $\Delta_{\min} = \Delta(1-\tilde{a}^2)^{1/2}$. At $\tilde{a}^2 > 1$ the shape of the FS near the touching points (see Fig. 3) does not lead to the discrete spectrum in the magnetic field, and formula (10) fails. With spectrum (10), we obtain at high magnetic fields $H \gg \bar{H} \equiv \max[H_T, H_T(\Delta\varepsilon_F)^2/T^2, H_T(\Delta_{\min})^2/T^2]$ [26],

$$\chi_{zz}(H) = -\frac{3f_0}{2^{5/4}\pi^2}\frac{e^{7/4}(b_{xx}b_{yy})^{3/8}(1-\tilde{a}^2)^{9/8}}{c^{7/4}\hbar^{5/4}|B|^{1/2}H^{1/4}}, \qquad (11)$$

where $f_0 \approx 0.156$. Expression (11) can also be rewritten in the form $\chi_{zz}(H) = (9f_0/\sqrt{2})\chi^0_{zz}(\varepsilon_F)(\bar{H}/H)^{1/4}$ which reveals the H dependence of the diamagnetic peak magnitude and shows that the giant anomaly is suppressed in strong magnetic fields.

Finally, it is worth noting that the band-contact lines in crystals can, in principle, intersect each other, and at the points of their intersection more exotic electron topological transitions than the $3\frac{1}{2}$-order transitions considered here are possible. At some of these exotic transitions the magnetic susceptibility can exhibit unusual anomalies [27].

IV. CONCLUSIONS

We have theoretically studied the electron topological transitions of the $3\frac{1}{2}$ kind associated with band-contact lines in 3D metals. In the 3D metals with inversion symmetry and a weak spin-orbit interaction these transitions are widespread no less than the well-known $2\frac{1}{2}$-order transitions of Lifshits.

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