Upper critical magnetic field in superconducting Dirac semimetal

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Abstract – Temperature dependence of the upper critical field $H_{c2}$ of the Dirac semimetal (DSM) with phonon-mediated pairing is considered within the semiclassical approximation. The low-temperature dependence deviates from conventional BCS superconductor with parabolic dispersion relation (Werthamer N. R., Helfand E. and Hohenberg P. C., Phys. Rev., 147 (1966) 295; Helfand E. and Werthamer N. R., Phys. Rev. Lett., 13 (1964) 686) even for large adiabaticity parameter, $\gamma = \mu/\hbar \Omega$, where $\mu$ is the chemical potential and $\Omega$ the Debye frequency. In particular the “reduced field”, ratio of zero-temperature $H_{c2}$ to the derivative at critical temperature, $h^v = H_{c2}(0)/(-T \frac{dH_{c2}}{dT})|_{T_c}$, depends on $\gamma$ and can be extended beyond the adiabatic limit. The reduced magnetic field ratio is universal (independent of the chemical potential, interaction strength, etc.) and smaller than the Werthamer ratio for clean superconductors: $h^v(0) = 0.55$ for DSM, $h^v(0) = 0.69$ for parabolic band. The results are in good agreement compared with recent experiments on TaP.

Introduction. – Recently a large new class of 2D (including purely 2D materials like graphene and surfaces of “topological insulators”) and 3D multi-band materials with qualitatively different band structure (Dirac point) near the Fermi level was discovered. Unlike in conventional semimetals with several quasiparticle and hole bands, the Dirac points occur due to the band inversion near the Fermi level. In many of them (sometimes under pressure) superconductivity was observed at low temperatures [1–6]. Dirac semimetals (DSM) are characterized by linear dispersion relation, and the chemical potential is tunable and small. More importantly for the pairing of the quasiparticles by phonons leading to “conventional” superconductivity is that their inter-band tunneling is dominant [7,8].

In type-I DSM, the band inversion results in Dirac points in low-energy excitations being anisotropic massless “relativistic” fermions (Dirac cone in dispersion relation, $\varepsilon = vp$). They exhibit several remarkable properties like the chiral magnetic effect related to the chiral anomaly in particle physics and tend to form s-wave superconductivity [9–12] of the second kind (the recently discovered type-II DSMs [13,14] with tilted cones and nearly flat bands tend to exhibit superconductivity of first kind [5]).

The magnetic properties of the DSM turned to a superconductor of the second kind are typically standard. The upper critical magnetic field $H_{c2}(T)$ was measured in a wide range of temperatures for different DSM and it shows a behavior typical of vortex matter. In particular in the layered DSM (that possess relatively large Ginzburg number $G_0$) MoTe$_2$ [15] thermal fluctuations effects are observed in the vicinity of the critical temperature $T_c$ [16–18]. The general theory based on the Ginzburg-Landau approach (that is insensitive to the microscopic details distinguishing between metal with parabolic bands and DSM of high $T_c$ unconventional superconductors) is applicable for most of the observed features.

However it was noticed very recently that the low-temperature dependence of the $H_{c2}(T)$ curve in some DSM, like [19] ZrTe$_5$, [20] Cd$_3$As$_2$ and [21] TaP, significantly deviate from that predicted by the quasiclassical...
microscopic theory for conventional parabolic band superconductors \cite{22–24}. The low-temperature limit is beyond the universality range of the GL approach and is sensitive to the “microscopic details”, especially when the inter-band tunneling is present. The deviations were discussed in the literature for superconductors that have large gyromagnetic ratio \cite{25}, but this is clearly not the case here. Therefore it is important to extend the original Werhamer-Hefland-Hohenberg \cite{22} theory (WHH) of the upper critical field to the case of multi-band DSM with large tunneling between the valleys \cite{17,18,26}.

This is the purpose of the present work. The quasi-classic theory of the phonon-mediated pairing in magnetic fields in DSM is developed in a wide range of temperatures and adiabatic parameters. In particular the reduced magnetic field at zero temperature defined by $h^* = H_{\Omega}(0)/(-T_d h_\beta/4T)|_{T}$, for different adiabaticity ratio $\gamma = \mu / h \Omega$ (\(\mu\) is the chemical potential, while $\Omega$ is the Debye frequency) is calculated. Even within the BCS limit by Bulaevsky \cite{24} with the magnetic field directed perpendicular to the layers) value $h^*_{WHH} = 0.69$.

In addition, since in DSM the Weyl adiabaticity ratio is relatively small, an important additional issue is the role of the retardation effects of the phonon-mediated pairing. Within the semiclassical approach one can approach the moderately adiabatic case, $\gamma \simeq 1$.

Pairing in DSM under magnetic field. –

Hamiltonian. Dirac model typically possesses several sublattices. We exemplify the effect of the DSM band structure on superconductivity using the simplest model with just two sublattices denoted by $\alpha = 1, 2$. The effective electron-electron attraction due to the electron-phonon coupling overcomes the Coulomb repulsion and induces pairing. Typically in DSM there are numerous bands. We assume that different valleys are paired independently and drop all the valley indices (including chirality, multiplying the density of states by $2N_f$). To simplify notations, we therefore consider just one spinor (left, for definiteness), the following Weyl Hamiltonian \cite{8,27}:

$$K = \int_{\vec{r}} \left(\frac{\hbar^2}{2m}\nabla^2 \psi_{\alpha}^+ (\vec{r}) - i\hbar v_{\alpha} (D_x \sigma_{\alpha \beta}^x + D_y \sigma_{\alpha \beta}^y) \right. $$

$$\left. - i\hbar v_{z} (D_z \sigma_{\alpha \beta}^z - \mu \delta_{\alpha \beta}) \right) \psi_{\beta} (\vec{r}).$$ (1)

Here $v$ is Fermi velocity assumed isotropic in the $x$-$y$ plane perpendicular to the applied magnetic field, $v_z$ is the velocity in the magnetic field direction. The chemical potential is denoted by $\mu$. The Pauli matrices $\sigma$ operate in the sublattice space (\(\alpha, \beta\) will be termed the pseudo-spin projections) and the indices are the spin projection. The magnetic field appears in the covariant derivatives via the vector potential, $D_i = \nabla^i - i \frac{e}{\hbar c} A_i$. Here $A$ is the vector potential.

Further we assume the local density-density interaction Hamiltonian \cite{28},

$$V = \frac{g^2}{2} \int \psi_{\alpha}^+ (\vec{r}) \psi_{\alpha} (\vec{r}) \psi_{\beta}^+ (\vec{r}) \psi_{\beta} (\vec{r}),$$ (2)

ignoring the Coulomb repulsion (that as usual is accounted for by a pseudopotential, so that $g$ is the electron-phonon coupling). It is important that the interaction has a cutoff Debye frequency $\Omega$, so that it is active in an energy shell of width $2\Omega h$ around the Fermi level \cite{28}.

Matsubara Green’s functions and Gor’kov equations. The finite-temperature properties of the superconducting condensate are described by the normal and the anomalous Matsubara Green’s functions \cite{28} (GF),

$$G_{\alpha\beta}^{s, t} (i\omega_n, \vec{r}, \vec{r}') = \langle T\psi_{\alpha}^{s, t}(\vec{r}) \psi_{\beta}^{s, t}(\vec{r}') \rangle,$$

with the spin ansatz

$$G_{\alpha\beta}^{s} (i\omega_n, \vec{r}, \vec{r}') = \delta^{s,t} G_{\alpha\beta} (\vec{r}, \vec{r}', \tau, -\tau'),$$

$$G_{\alpha\beta}^{t} (i\omega_n, \vec{r}, \vec{r}') = -\delta^{s,t} F_{\alpha\beta} (\vec{r}, \vec{r}', \tau, -\tau'),$$

Here the Planck constant is set to $\hbar = 1$. Using the Fourier transform,

$$G_{\gamma\alpha}(\vec{r}, \vec{r'}) = T \sum_s \exp[-i\omega_s \tau] G_{\gamma\alpha}(\omega, \vec{r}),$$ (5)

with fermionic Matsubara frequencies, $\omega_s = 2\pi T (s+1/2)$, one obtains from the equations of motion of the operator the set of Gor’kov equations, see \cite{8,29} generalized to include the magnetic field:

$$(i\omega + \mu) G_{\gamma\alpha}(\vec{r}, \vec{r}', \omega) + i \hbar D_i \sigma_{\gamma\beta}^i G_{\beta\alpha}(\vec{r}, \vec{r}', \omega) + \Delta_{\gamma\alpha}(\vec{r}, 0) F_{\beta\alpha}^{\dagger}(\vec{r}, \vec{r}', \omega) = \delta^{\gamma\nu}\delta(\vec{r} - \vec{r}')$$

$$(i\omega + \mu) F_{\gamma\alpha}(\vec{r}, \vec{r}', \omega) - i \hbar D_i \sigma_{\gamma\beta}^i F_{\beta\alpha}^{\dagger}(\vec{r}, \vec{r}', \omega) - \Delta_{\gamma\alpha}(\vec{r}, 0) G_{\beta\alpha}(\vec{r}, \vec{r}', \omega) = 0.$$ (6)

It will be shown that the singlet pairing pseudo-spin ansatz, $\Delta_{\gamma\alpha} \equiv \sigma_{\gamma\alpha}^x \Delta$, obeys the Pauli principle. The gap function consequently reads: $\Delta = \frac{\Delta}{2} \Gamma[\pi (\sigma^2 \Delta)]$. Notice, that in contrast to conventional metals with parabolic dispersion law, in the case of the Weyl semimetals the second Gor’kov equation, eq. (6), contains transposed Pauli matrices for isospins. The applicability of the mean-field approach in a purely 2D model has been widely discussed \cite{30} since (logarithmic) infrared divergences appear in corrections to the approximation. The corrections of the long-range charge density waves instability are assumed to be cut off by the finite size of the sample, etc.
The transition line in the H-T plane. – Near the normal-to-superconducting transition line the gap $\Delta$ is small and the set of the Gor’kov equations (6) can be linearized. We consider here the 2D case neglecting motion in the magnetic field direction. A more general case will be discussed below. In this case the gap equation describing the critical curve $H_c2(T)$ has the form, see [29] for details,

$$\Delta(r) = \frac{g^2}{2} \sum_{\omega} \int_{r'} \Delta^*(r') \sigma_{\gamma\beta} G_{\beta \gamma}^2(r', r) \sigma_{\gamma\alpha} G_{\alpha \gamma}^1(r, r')$$

where $G_{\beta \gamma}$ (an auxiliary function associated with $G$ via a product of an axis reflection and time reversal) obeys different equation:

$$[\imath \omega \mathbf{D}_r \cdot \sigma_{\gamma\beta} + (\imath \omega + \mu) \delta_{\gamma\beta}]G_{\beta \gamma}^1(r, r') = \delta^{\gamma\beta} \delta(r - r').$$

Here $\sigma^\dagger$ is the transpose Pauli matrix that replaces $\sigma$ in the customary normal-state Weyl equation for left movers, eq. (8).

In the uniform magnetic field the GF can be written in the symmetric gauge, $\mathbf{A} = -\frac{1}{2} \mathbf{H} \times \mathbf{r}$, in the following form:

$$G_{\beta \gamma}^1(r, r') = \exp \left[ -\frac{\imath y (x' - y')}{2l^2} \right] g_{\beta \gamma}^1(r - r'),$$

$$G_{\beta \gamma}^2(r', r) = \exp \left[ -\frac{\imath y (x - y')}{2l^2} \right] g_{\beta \gamma}^2(r' - r).$$

Here $l^2 = c/eh$ is the magnetic length. This phase ansatz indeed works. Substituting it into eq. (8) and eq. (9), respectively, the variables separate. It reads

$$L_{\gamma\beta}^1 g_{\beta \gamma}^1(r - r') = \delta^{\gamma\beta} \delta(r - r'),$$

$$L_{\gamma\beta}^2 g_{\beta \gamma}^2(r' - r) = \delta^{\gamma\beta} \delta(r' - r),$$

where $L_{\gamma\beta}^1 = [i\omega + \mu] \delta_{\gamma\beta} + (-\imath v \sigma_{\gamma\beta} \nabla_r)$, $L_{\gamma\beta}^2 = [(-\imath \omega + \mu) \delta_{\gamma\beta} - \imath v \sigma_{\gamma\beta} \nabla_r]$. Solutions of these equations give

$$g_{\gamma\beta}^1(p) = z^{z-1}(i\omega + \mu), \quad g_{\gamma\beta}^1(p) = -z^{z-1}(i\omega + \mu),$$

$$g_{\gamma\beta}^2(p) = -z^{z-1}(i\omega + \mu), \quad g_{\gamma\beta}^2(p) = z^{z-1}(i\omega + \mu),$$

$$g_{\gamma\beta}^2(p) = -z^{z-1}(i\omega + \mu), \quad g_{\gamma\beta}^2(p) = z^{z-1}(i\omega + \mu),$$

where $z = (-\imath \omega + \mu)^2 - (vp)^2$ and $p$ denote quasimomentum.

Substituting the phase factors of GF from eq. (10) into the gap equation, eq. (7), one obtains

$$\Delta(r) = g^2 T \sum_{\omega} \int_{r'} \exp \left( \frac{\imath r \cdot \rho}{l^2} \right) \Delta^*(r')$$

$$\times [g_{\beta\gamma}^1(-\rho) g_{\beta\gamma}^2(\rho) + g_{\beta\gamma}^2(-\rho) g_{\beta\gamma}^1(\rho) + g_{\gamma\beta}^2(-\rho) g_{\gamma\beta}^1(\rho),$$

where $\rho = r - r'$. Looking for the gap function $\Delta(r)$ in the form [31] $\Delta(r) = \Delta \exp(-r^2/2\pi^2)$, one obtains after Fourier transformation

$$S(p, q) = \frac{2 \omega^2 + \mu^2 + v^2(p - q) \cdot p}{[(i\omega + \mu)^2 - v^2(p - q)^2][(i\omega + \mu)^2 - v^2p^2]}.$$

In polar coordinates, eq. (14) has the form

$$S(p, q) = \exp \left( \frac{\rho^2}{2l^2} \right) \int \frac{d^2p d^2q}{(2\pi)^4} e^{i\mathbf{p} \cdot \mathbf{q}} S(p, q),$$

where

$$S(p, q) = \frac{2 \omega^2 + \mu^2 + v^2(p - q) \cdot p}{[(i\omega + \mu)^2 - v^2(p - q)^2][(i\omega + \mu)^2 - v^2p^2]}.$$
\[ \lambda = \frac{2\chi}{\mu} \sum_{\omega} \int d\varepsilon_p d\varepsilon_q d\psi \frac{f(\varepsilon_p)\varepsilon_q\varepsilon_p \exp[-\chi\varepsilon_q^2] (\varepsilon_p^2 + \varepsilon_q^2 + \varepsilon_p^2 - \varepsilon_q^2 \cos \psi)}{((-i\varepsilon + \mu)^2 - (\varepsilon_p^2 + \varepsilon_q^2 - 2\varepsilon_p\varepsilon_q \cos \psi))^{1/2}}. \]  

(18)

Fig. 1: (Color online) Upper critical field as a function of temperature for various adiabatic ratio \( \gamma \) and electron-electron strength \( \lambda \) values: (a) \( \gamma = 10 \), (b) \( \gamma = 3 \), (c) \( \gamma = 1 \). Dashed lines are described by the universal interpolation formula (19) with reduced magnetic field \( h^* = 0.55 \) parameter. Color scale marks \( \lambda^{-1} \) magnitudes.

interaction due to phonon exchange, so the sharp cutoff might be replaced by the “smooth” Lorenzian function

\[ f(\varepsilon_p) = \frac{\Omega^2}{\Omega^2 + (\varepsilon_p - \mu)^2}. \]  

(17)

Performing the integral [17,32] over the angle \( \Theta \) and \( \rho \), one obtains the coexistence curve in the \( H-T \) plane in reduced variables with barred energies denoting division by temperature \( T \):

see eq. (18) above

Here \( \lambda = D(\mu)g^2 \) is the electron-electron strength constant, \( D(\mu) = \mu/4\pi v^2 \) is the density of free 2D Dirac electron gas. The dimensionless magnetic field parameter in the exponent is defined by \( \chi = c\sqrt{\bar{h}/v}/2e\ell^2h \), where \( t \equiv T/\Omega, t_c = T_c/\Omega \). Performing the summation over Matsubara frequencies and numerical integrations, one obtain the upper critical magnetic fields depending on temperature and adiabaticity parameter \( \gamma = \mu/(\hbar\Omega) \).

In fig. 1 the magnetic field is given in units of magnetic field \( H_u = \Omega^2/(\pi v)^{3/2} \) for three different values of the adiabaticity parameter \( \gamma \) and the DSM superconductors electron velocity \( v = 10^7 \text{cm/s} \), typical of these materials. The temperature dependence \( H'_{C2}(T) \) is fitted very well by an interpolation formula,

\[ H(T) = H(0)(1 - (T/T_c)^{1/h^*}), \]  

(19)

for the universal value of the reduced magnetic field \( h^* = 0.55 \) determining the exponent. Results of the theory demonstrate excellent agreement with the temperature dependence of the upper critical magnetic field measured in the DSM TaP [21], see fig. 2.

In a more general case when motion in the \( z \)-axis direction (parallel to the magnetic field) \( v_z \) is not zero, the upper critical field does not depend on \( v_z \), since it renormalized the density of states and hence the electron-electron strength constant. The reduced magnetic field \( h^* \) in this case coincides with that calculated for layered system (similar to conventional superconductors [24]).

Conclusions. – In this paper, the microscopic semiclassical theory of phonon-mediated superconductivity in Dirac semimetals under magnetic fields was constructed in entire range of temperature. The main results
are presented in figs. 1, 2. Within the weak-coupling approach, the retardation effects were explicitly taken into account by the dispersionless model of the electron-phonon coupling, eq. (17). This is of importance since commonly used step function produce spurious oscillation [18,30].

The upper critical magnetic field $H_{c2}$ is lower than predicted by the conventional Werthamer-Helfand-Hohenberg formula [22] derived for superconductors with parabolic dispersion relation. The reduced magnetic field ratio is universal (independent of the chemical potential, interaction strength etc.) and smaller than the Werthamer ratio $h^* = H_{c2}(0)/(-T\frac{\partial H_{c2}}{\partial T})|_{T_c}$ for clean superconductors: $h^* = 0.99$ for WSM, $h^*(0) = 0.69$ for parabolic band. This explains the recent experiments on Cd$_3$As$_2$, ZrTe$_5$ and especially on TaP (see refs. [20], [3] and [21], respectively). Going beyond the semiclassical approximation is typically more complicated and has been contemplated in parabolic band materials [31] and recently in Weyl semimetals [18,33].

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