Superconducting critical temperature and upper magnetic field in Weyl semimetal.

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Abstract. The influence of recently discovered topological transition between type I and type II Weyl semi-metals on superconductivity is considered. A set of Gorkov equations for weak superconductivity in Weyl semi-metal under topological phase transition is derived and solved. The critical temperature has spike in the point the transition point as function of the tilt parameter of the Dirac cone determined in turn by the material parameters like pressure. The second critical magnetic field is calculated for phase I. It shows narrow domains of reentrant superconductivity associated with Landau quantization relativistic 2D electron gas.

1. Introduction

Recently new class of 2D and 3D Weyl semi-metals were discovered. Most of them are characterized by linear dispersion relation near the Fermi surface (Dirac cone). The first material of this class, graphene\cite{1}, exhibits the highest symmetry leading to linear ultra - relativistic spectrum, however most of the other materials are anisotropic. Examples include 2D Weyl semi-metals (WSM) silicene, germanene and borophene \cite{2} and 3D crystals\cite{3} \textit{Na}_3\textit{Bi} , and\cite{4} \textit{Cd}_3\textit{As}_2 and numerous layered organic compounds\cite{5, 6, 7}. Topological insulators (TI) like \textit{Bi}_2\textit{Se}_3 and other \cite{8} generally have Dirac cones on their surfaces of topological insulators.

The pressure modifies the spin orbit coupling that in turn determines the topology of the Fermi surface of these novel materials \cite{9}. Very recently the topological transition in Weyl semi - metal under pressure was observed \cite{10}.

Some Weyl materials are known to be superconducting. A detailed study of superconductivity in TI under hydrostatic pressure revealed a curious dependence of critical temperature of the superconducting transition on pressure \cite{11} . In intercalated \textit{Sr}_{0.065}\textit{Bi}_2\textit{Se}_3 single crystal \cite{12} considered to be a pure material ambient weak superconductivity first is suppressed, but at high pressure of \textit{6GPa} reappears and reaches relatively high \( T_c \) of \textit{10K} that persists till \textit{80GPa}. The increase is not gradual, but rather abrupt in the region of \textit{15GPa} \cite{12}. Superconductivity in similar TI compounds \cite{13, 14, 15} \textit{Bi}_2\textit{Se}_3 , \textit{Bi}_2\texti{T}_e\textsubscript{3} and 3D Weyl semi-metal\cite{16} \textit{HfTe}_5 were also studied experimentally. The critical temperature \( T_c \) in some of these systems shows a sharp maximum as a function of pressure. Various mechanisms of superconductivity in Dirac semi – metals and topological insulators turned superconductors have been considered theoretically \cite{17, 18, 19}. A theory predicted possibility of superconductivity in the type II Weyl semimetals was developed recently in the framework of Eliashberg model \cite{20}.
We calculated in this paper the critical temperature for arbitrary tilt and find its sharp increase at topological transition point from type I to type II Weyl semi-metal. The critical second magnetic field $H_{c2}(T)$ was calculated for type-I semi metals. It shows narrow domains of reentrant superconductivity associated with Landau quantization relativistic 2D electron gas.

2. Type I and type II Weyl semi-metal with local pairing interaction.

Weyl material typically possesses several sublattices. We exemplify the effect of the topological transition on superconductivity using the simplest possible model with just two sublattices denoted by $α = 1, 2$. The band structure near the Fermi level of a 2D Weyl semi-metal is well captured by the following Hamiltonian,

$$
K = \int r \psi^L_{α}(r) K^L_{αβ}(r) \psi^L_{β}(r) + \psi^R_{α}(r) K^R_{αβ}(r) \psi^R_{β}(r);
$$

$$
K^L,R_{αβ} = -iμv \left( \nabla \cdot \sigma^α_{αβ} + \nabla \cdot \sigma^β_{αβ} \right) + (-iμw - μ) δ_{γδ}.
$$

Here $v$ is Fermi velocity, $μ$ - chemical potential, $γ$ are Pauli matrices in the sublattice space and $s$ is spin projection. We restrict ourselves to the case of just one left handed ($L$) and one right handed ($R$) Dirac points, typically but not always separated in the Brillouin zone. The 2D velocity vector $w$ defines the tilt of the cone. The effective electron-electron attraction due to either electron - phonon attraction and Coulomb repulsion (pseudopotential) or some unconventional pairing mechanism creates pairing. We assume that different valleys are paired independently and drop the valley indices (multiplying the density of states by $2N_f$). Further we assume the local singlet s-channel interaction Hamiltonian

$$
V = \frac{g^2}{2} \int dr \, \psi^α_α(r) \psi^α_β(r) \psi^β_α(r) \psi^β_β(r).
$$

As usual the interaction has a cutoff frequency $Ω$, so that it is active in an energy shell of width $2ħΩ$ around the Fermi level [21]. For the phonon mechanism it is the Debye frequency.

3. Gor’kov Green functions.

Finite temperature properties of the superconducting condensate are described by the normal and the anomalous Matsubara Greens functions [21]:

$$
G^{ts}_{αβ}(r, r′; τ') = δ^{ts} g_{αβ}(r, r′, τ - τ'); F^{ts}_{αβ}(r, r′; τ') = -δ^{ts} f_{αβ}(r, r′, τ - τ'); F^{tt+ts}_{αβ}(r, r′; τ') = δ^{tt+ts} f_{αβ}(r, r′, τ - τ')
$$

Using the Fourier transform, $g_{ργ}(ω, r) = T \sum_{ω} \exp[-iωτ]g_{ργ}(ω, r)$, with Matsubara frequencies, $ω_n = 2πT(n + 1/2)$, one obtains from equations of operator motion the set of Gor’kov equations [22]

$$
iωg_{ργ}(r, r', ω) - iνσ^ρ γ β \nabla_r g_{γ δ}(r, r', ω) + μg_{ργ}(r, r', ω) + Δ_{αγ}(r, 0) f^+'_{αγ}(r, r', ω) = δ^{ργ}δ(r - r')
$$

$$
- iωf^+_{ργ}(r, r', ω) - iνσ^ρ γ γ \nabla_r f^+_{ργ}(r, r', ω) + μf^+_{ργ}(r, r', ω) - Δ^*_{αγ}(r, τ = 0) g_{αγ}(r, r', ω) = 0
$$

Here $Δ_{αγ} ≡ σ^α γ Δ$, $Δ = τ^2 Δ^γ γ$ is the gap Ansatz in s-wave channel, indexes $t, s$ and $α, β$ relate to spin and pseudospin.

In matrix form (in sub-lattice space) we obtain the solution in uniform case [22]

$$
\tilde{G}(ω, p) = σ^γ (p ∙ σ^γ + (-iω + μ - wp)x) M^{-1}; \tilde{f}^+(ω, p) = M^{-1} Δ^+, \hspace{1cm} \text{where}
$$

$$
M = (vp ∙ σ + (iω + μ - wp)x) I σ^γ (vp ∙ σ^γ + (-iω + μ - wp)x) I + |Δ|^2 σ^γ,
$$

and $I$ is the identity matrix.
4. Critical temperature.

The gap as function of the material parameters is determined by the gap equations

\[ \Delta^* = \frac{\Delta^*}{2(2\pi)^3} T \sum_\omega d\mathbf{p} \text{Tr}[\sigma_x M^{-1}], \]  

The critical temperature is defined from the gap equation, when the gap \( \Delta \) vanishes:

\[ T_c = 1.14\Omega \exp\left[-\frac{1}{\lambda f(\kappa)}\right], \]

The function \( f(\kappa) \) reads

\[ f(\kappa) = \begin{cases} 
\frac{2\kappa^2}{(1-\kappa^2)^{3/2}} & \text{for } \kappa < 1 \\
\frac{2\sqrt{1+\kappa} - 1 + \log \frac{2(\kappa^2-1)}{\kappa(1+\sqrt{1+\pi})}}{\delta} & \text{for } \kappa > 1 
\end{cases}, \]

where \( \kappa = w/v \) is the anisotropy parameter, \( \delta = \pi a\Omega/v\hbar \) is the cutoff parameter, \( a \) is the interatomic distance. (The effective density of states \( f(\kappa) \) formally diverges at \( \kappa = 1 \). It’s result of linear dispersion relation in the model Weyl Hamiltonian. Indeed, the linear approximation of the dispersion relation in the Weyl semimetal is valid only for small neighborhood of the Dirac point. At higher energies the band spectrum is nonlinear and cut off by the band width \( 1/a \). Fig.1 demonstrates that the critical temperature has a sharp spike at the transition point \( w = v \). The ratio \( \frac{2\Delta}{T_c} \) is still universal for any \( w/v \). (Similar results were obtained in Ref [20] for small and large cone tilt).
5. Critical Magnetic Field

If the superconductor is subjected to external magnetic field $H$ then the gap equation $H_{c2}(T)$ has the form

$$\Delta(r) = \frac{g^2}{2} T \int \int \Delta^*(r') \sigma_{\alpha \beta} G_{\beta \gamma}(r, r') \sigma_{\gamma \alpha} G_{\alpha \delta}(r', r)$$

(11)

where $G_{\alpha \beta}(r, r')$ and $G_{\beta \gamma}(r, r')$ are the Green functions of the normal state obeying the equations:

$$\left\{ \begin{array}{l}
-v \left( -i \nabla - \frac{e}{c} A \right) \cdot \sigma_{\gamma \beta} + (i \omega + \mu) \delta_{\gamma \beta} \right\} \sigma_{\beta \delta} G_{\beta \delta}(r, r') = \delta^{\gamma \delta} \delta(r - r') \\
-v \left( -i \nabla - \frac{e}{c} A \right) \cdot \sigma_{\gamma \beta} + (-i \omega + \mu) \delta_{\gamma \beta} \right\} \sigma_{\beta \delta} G_{\beta \delta}(r, r') = \delta^{\gamma \delta} \delta(r - r')
\end{array} \right. 
$$

(12)

(13)

Here $\sigma^\dagger$ is the transposed Pauli matrix. In the uniform magnetic field the Green's functions can be written in the Ansatz form:

$$G_{\beta \delta}^1(r, \rho, \omega) = \exp \left( \pm \frac{e}{c} A(R, \rho) \right) g_{\beta \delta}^1(\rho, \omega)$$

(14)

where $R = \frac{r + r'}{2}, \rho = r - r'$. The vector potential in the symmetric gauge reads $A(r) = \frac{1}{4} (-Hy, Hx, 0)$. Substituting this Ansatz into Eqs.(12),(13) one obtains:

$$\left\{ \begin{array}{l}
(i \omega + \mu) \delta_{\gamma \beta} + v \sigma_{\gamma \beta} x + v \sigma_{\gamma \beta} y \right\} \sigma_{\beta \delta} g_{\beta \delta}(\rho, \omega) = \delta^{\gamma \delta} \delta(\rho) \\
(-i \omega + \mu) \delta_{\gamma \beta} + v \sigma_{\gamma \beta} x + v \sigma_{\gamma \beta} y \right\} \sigma_{\beta \delta} g_{\beta \delta}(\rho, \omega) = \delta^{\gamma \delta} \delta(\rho)
\end{array} \right. 
$$

(15)

(16)

are the Ladder operators related to creation and annihilation operators for bosonic field $a = \frac{1}{\sqrt{2}} (\Pi_x - i \Pi_y); a^+ = \frac{1}{\sqrt{2}} (\Pi_x - i \Pi_y); l = \sqrt{\frac{\Omega}{\gamma}}$ where $l$ is the magnetic length.

Solving the set of the equations (15) and (16) in polar coordinates and one performing summation on Matsubara frequencies one obtains [23] the equation for $H_{c2}$

$$\frac{1}{\lambda} = \frac{\omega^2}{4\pi^2} \left\{ \sum_{n,m=1}^{m+n+1} \frac{f[n] f[m]}{m! n!} s + \sum_{n=1}^{m+n+1} \frac{f[n] f[0]}{2^n} s_0 + \frac{f[0]^2}{2} s_{00} \right\}$$

(19)

where

$$f(n) = \frac{\Omega_D^2}{\Omega_D^2 + (\omega \sqrt{n - m})^2}$$

(18)

$$\omega_c \rightarrow \omega_c/T; \frac{\omega_c}{2} \rightarrow \mu/T; \frac{\Omega_D}{2} \rightarrow \Omega_D/T; \omega_c = \nu \sqrt{\frac{2}{l}}$$

are the reduced cyclotron frequency, chemical potential and Debye frequency correspondingly. Here $\lambda = \frac{\sqrt{\nu \mu}}{4 \pi} \tau_{ee}$ is the dimensional electron-electron constant for 2D electron gas (per sublattice).

$$s = (A \frac{1}{\omega_c^2} (n+1) \frac{1}{\omega_c^2} (m+1) + A \frac{2}{\omega_c^2} (n+1) \frac{2}{\omega_c^2} (m+1) + \mu^2 B \frac{1}{\omega_c^2} (n+1) \frac{2}{\omega_c^2} (m+1) + \mu^2 B \frac{1}{\omega_c^2} (n+1) \frac{1}{\omega_c^2} (m+1) + \mu^2 B \frac{1}{\omega_c^2} (n+1) \frac{2}{\omega_c^2} (m+1) + \mu^2 B \frac{1}{\omega_c^2} (n+1) \frac{1}{\omega_c^2} (m+1) )$$

(20)

(21)

$$s_0 = A \frac{1}{\omega_c^2} (n+1) + A \frac{2}{\omega_c^2} (n+1) + \mu^2 B \frac{1}{\omega_c^2} (n+1) + \mu^2 B \frac{1}{\omega_c^2} (n+1)$$

(22)

$$s_{00} = A \frac{1}{\omega_c^2} (n+1) + A \frac{2}{\omega_c^2} (n+1) + \mu^2 B \frac{1}{\omega_c^2} (n+1) + \mu^2 B \frac{1}{\omega_c^2} (n+1)$$
Figure 2. The upper critical field versus temperature. The figure is plotted for $\mu/\Omega_D = 5$. Domains of reentering superconductivity is presented for two different electron-electron strength $\lambda = 1$ (short light) and $\lambda = 0.66$ (long).

where

$$A[a,b] = \frac{(\sqrt{a} - \mu)^2 \tanh\left(\frac{\sqrt{a} - \mu}{2}\right)}{4\sqrt{a}(-b + (\sqrt{a} - 2\mu)^2)} + \frac{(\sqrt{b} - \mu)^2 \tanh\left(\frac{\sqrt{b} - \mu}{2}\right)}{4\sqrt{b}(-a + (\sqrt{b} - 2\mu)^2)} + \frac{(\sqrt{a} + \mu)^2 \tanh\left(\frac{\sqrt{a} + \mu}{2}\right)}{4\sqrt{a}(-b + (\sqrt{a} + 2\mu)^2)} + \frac{(\sqrt{b} + \mu)^2 \tanh\left(\frac{\sqrt{b} + \mu}{2}\right)}{4\sqrt{b}(-a + (\sqrt{b} + 2\mu)^2)}$$

(22)
Our result might provide an explanation of a spike in dependence of the upper critical magnetic field $H_{c2}$ on pressure in single crystals observed in many superconducting semi-metals [13, 14]. Due to small number of carriers in this semimetal, the quasiclassical Werthamer-Helfand approximation breaks down and Landau quantization is resonantly enhanced at the magnetic fields corresponding to full occupancy of the Landau levels in the shallow band. This enhancement is especially pronounced for the lowest Landau level. As a consequence, the reentrant superconducting regions in the temperature-field phase diagram emerge at low temperatures near the magnetic fields at which the chemical potential matches the Landau levels.

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\[ B[a,b] = -\frac{\tanh\left(\frac{\sqrt{a} - \pi}{2}\right)}{4\sqrt{a}(-b+(\sqrt{a} - 2\pi)^2)} - \frac{\tanh\left(\frac{\sqrt{b} - \pi}{2}\right)}{4\sqrt{b}(-a+(\sqrt{b} - 2\pi)^2)} \]

\[ -\frac{\tanh\left(\frac{\sqrt{a} + \pi}{2}\right)}{4\sqrt{a}(-b+(\sqrt{a} + 2\pi)^2)} - \frac{\tanh\left(\frac{\sqrt{b} + \pi}{2}\right)}{4\sqrt{b}(-a+(\sqrt{b} + 2\pi)^2)} \]