The Density of Surface States in Weyl Semimetals

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Weyl semimetal is a three-dimensional material with a conical spectrum near an even number of point nodes, where two bands touch each other. Here we study spectral properties of surface electron states in such a system. We show that the density of surface states possesses a logarithmic singularity for the energy $\varepsilon \to 0$. It decreases linearly at the intermediate energy of surface electron states and approaches zero as $\sqrt{1-\varepsilon}$ for $\varepsilon \to 1$. This universal behavior is a hallmark of the topological order that offers a new wide range of applications.

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Introduction.— New classes of matter known as topological insulators and Weyl semimetals are characterized by the linear dispersion of low-energy electron excitations on the surface and in the bulk, respectively. The states on the surface of these so-called Dirac materials have a fixed spin orientation for each momentum. The electron states in topological insulators [1–3] are topologically ordered and protected by the time-reversal symmetry. A condition for the existence of Weyl semimetal is breaking of either inversion or time-reversal symmetry. The topological order manifests itself as massless Dirac modes propagating along the edge or the surface of topological insulators or in the bulk of Weyl semimetals. Study of the properties of surface electron states, being a hallmark of the topological order, enables one to clarify some features of the topological order in the bulk. It should be noted that the topological classification [4,5] of phase states in topological insulators has been extended to Weyl semimetals [6]. The transport features of Weyl semimetals [3, 10] related to the chiral anomaly as well as the spectrum of collective excitations [11, 12] were recently studied (see reviews [13, 14]). Oscillations of the density of bulk states in Weyl semimetals in a strong magnetic field and their experimental signatures have been analyzed in Ref. [15].

In this paper, we examine the properties of Weyl semimetals when the time-reversal symmetry is preserved, while the spatial inversion symmetry is broken [16], focusing on the density of surface states. This type of Weyl semimetal is studied in Ref. [17] in which the spectrum of surface states is obtained. It has the form

$$E(k_x, k_y) = 4t \sin \frac{k_x a}{4} \sin \frac{k_y a}{4}$$

and is shown in Fig. 1. Here $\mathbf{k} = (k_x, k_y)$ is the two-dimensional wave vector, $t$ is the integral of nearest-neighbor hopping, and $a$ is the lattice constant.

Density of surface states.— The density of surface states is defined by the integral over the surface Brillouin zone (BZ) $|k_x \pm k_y| \leq \frac{\pi}{a}$ of the delta function $\delta[E - E(k_x, k_y)]$ as follows

$$N(E) = \int_{BZ} \frac{d^2 k}{(2\pi)^2} \delta[E - E(k_x, k_y)].$$

Having introduced the dimensionless quantities, i.e., the density of surface states $n(\varepsilon) = N(E)/N_0$ with $N_0 = 4/((\pi^2 a^2)t)$, the energy $\varepsilon = E/(2t)$, the wave vector components $(x, y) = (k_x a/4, k_y a/4)$, after the change of variables $\xi = x - y$, $\eta = x + y$, we obtain

$$n(\varepsilon) = \frac{1}{4} \int_{-\pi/2}^{\pi/2} d\xi \int_{-\xi}^{\xi} d\eta \delta[\varepsilon - \cos \xi + \cos \eta] =$$
FIG. 2. The density of surface states $n(\varepsilon)$ vs. the energy $\varepsilon$ in Weyl semimetal.

The knowledge of $N(\varepsilon)$ and the value $N(\varepsilon_F)$ at the Fermi energy $\varepsilon_F$ is important for studying the internal electrostatic effects and the external gate-voltage effects [21]. The quantum capacitance $C_Q$ per unit area of a two dimensional system is given, e. g., by $C_Q = e^2 N(\varepsilon_F)$, where $e$ is the electron charge. This could be used for experimental check of the features of the density of surface states in Weyl semimetals. The density of states also determines the dc conductivity $\sigma_{dc}$. Einstein’s formula $\sigma_{dc} = e^2 N(\varepsilon_F) D$ expresses $\sigma_{dc}$ in terms of the density of states and the diffusion constant $D = v_F^2 \tau$, where $\tau$ is the transport lifetime. Obviously, we have thereby a contribution of the surface conductivity to the total one in tunneling in Weyl semimetals. As for the distribution of spin degrees of freedom, bulk states for one Dirac node in Weyl semimetal resemble chiral quasi-spin configurations in graphene, while surface states in Weyl semimetal are analogs of helical distributions of spin directions in topological insulators. The energy spectrum and the spin texture of surface states can be experimentally studied using the tunneling spectroscopy technique, for which the behavior of the density of surface states is the key one.

In conclusion, we have calculated the density of surface states in Weyl semimetals and have shown that it possesses the logarithmic singularity for $\varepsilon \to 0$ decreasing linearly at the intermediate energy of surface electron states and approaching zero as $\sqrt{1 - \varepsilon}$ for $\varepsilon \to 1$. It resembles the behavior of the set of two orthogonal one-dimensional Dirac metals embedded in two-dimensional space.

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