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ACCEPTED MANUSCRIPT

Optical transitions in two-dimensional topological insulators with point defects

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Abstract

Nontrivial properties of electronic states in topological insulators are inherent not only to the surface and boundary states, but to bound states localized at structure defects as well. We clarify how the unusual properties of the defect-induced bound states are manifested in optical absorption spectra in two-dimensional topological insulators. The calculations are carried out for defects with short-range potential. We find that the defects give rise to the appearance of specific features in the absorption spectrum, which are an inherent property of topological insulators. They have the form of two or three absorption peaks that are due to intracenter transitions between electron-like and hole-like bound states.

Keywords: topological insulator, impurities, bound states, optical absorption *PACS:* 71.55.-i, 73.20.-r, 78.67.-n

1. Introduction

Topological quantum states arising in topological insulators (TIs) due to strong spin-orbit interaction and time reversal symmetry attract a great deal of interest because of their nontrivial properties as well as because they provide us with opportunities to explore qualitatively new physical phenomena challenging for construction of novel quantum devices, spintronic applications and topological quantum computation [1–3]. The topological states are robust since they are protected against the scattering by weak non-magnetic impurities and disorders. The main attention is paid to topological states that exist near the surface of three-dimensional TIs and the edge of two-dimensional (2D) TIs. However, unusual electron states arise also at impurities and structure defects located in the bulk.

Impurity induced states were studied both for impurities on the surface of three-dimensional TIs [4, 5, 7–9], and in 2D TIs [10–14]. In addition, the impurity states were discussed for one-dimensional topological systems [12]. The main conclusion is that the electron density localizes near the defect in a highly unusual way. A similar phenomenon can occur in a trivial one-dimensional system with spin-orbit interaction in the presence of a weak magnetic field [15].

In the present paper we address to the 2D TIs since many experiments presently indicate the important role of structural defects in these materials, especially in the electron transport. Theoretical studies of bound states induced by nonmagnetic defects in the bulk of 2D TIs have revealed specific properties of these states which are in-

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herent to 2D TIs and absent in the topologically trivial crystals.

It turns out that in 2D TIs there are two mechanisms of the bound state formation in contrast to the trivial case where a bound state arises only as a quasiparticle (electron or hole) is localized in a quantum well produced by the defect. In 2D TIs, bound states are formed by the repulsive potential as well. These states are similar to the helical edge states at the boundary of the 2D TI. Their distinguishing feature is that the electron density is low in the center but concentrated around the defect. Correspondingly there are two kinds of the states located at the defect. In particular, a defect with strongly localized potential induces two states irrespective of the sign of its potential. This contrasts to the trivial case where the same defect produces only one state. It is worth noting that two states located at a given defect are distinguished also by their pseudospin structure. In one state, the hole component of the spinor equals zero in the center while in the other state, the electron component turns to zero there. Correspondingly the states can be classified also as the electron-like and hole-like states [14, 16].

In experiments, the defect-induced bound states are still poorly understood though they attract continuously increasing interest, which is stimulated mainly by discrepancies between the experiments and expectations of the theory. The discrepancies are usually associated with the presence of uncontrolled defects, the density of which is apparently high under the real conditions.

In particular, the electric conductance of the edge states in experiments [17–22] appears to be smaller than the universal quantity e^2/h predicted by the existing theories [1]. It turns out that in many experiments [19–22] the conductance is decreased by several times or even orders of

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