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Variable resistance at the boundary between semimetal and excitonic insulator

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Abstract

We solve the two-band model for the transport across a junction between a semimetal and an excitonic insulator. We analyze the current in terms of two competing terms associated with neutral excitons and charged carriers, respectively. We find a high value for the interface resistance, extremely sensitive to the junction transparency. We explore favorable systems for experimental confirmation.

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1. Introduction

The concept that excitons can condense in a semimetal (SM) and form an *excitonic insulator* (EI), if the energy band overlap is small compared to their binding energy, dates back to the sixties [1]. Experimental evidence has been put forward for the exciton phase [2], but the EI state remains a mystery. Moreover, the possibility of experimental discrimination between the EI and the ordinary dielectric has been called into question [3]. We demonstrate that, if an EI exists, it develops unusual transport properties that make it qualitatively different from an ordinary insulator.

Elsewhere [23], we considered, in a two-band model, a junction between a SM and a semiconductor, whose small gap originates from the renormalization of the SM energy bands due to: (i) hybridization of conduction and valence bands, (ii) electron–hole pairing driving the EI condensation. Carriers incident on the interface from the SM side

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with energies below the gap are backscattered again into the SM, possibly into a different band. We found that interband scattering only occurs for (ii), due to the proximity of the EI which broadens the interface potential profile.

Here we focus on the latter case only. We analyze the current generated by a bias voltage across a clean SM/EI junction as two competing terms associated with neutral excitons and charged carriers, respectively. Below the EI gap, carriers are backscattered by the interface with energy band branch crossing. The formalism is similar to that for the metal/superconductor (NS) interface [4], and indeed we find the same dependence of transmission and reflection coefficients on the quasi-particle energy ω . However, while electrons below the superconducting gap are Andreevreflected as holes, carriers reflected below the EI gap conserve their charge and the electric current is zero. Above the gap, when charge transmission is allowed, an unusually high electrical resistance remains. We find that the electrons that are backscattered from one band to another are equivalent to incoming holes correlated with the incoming electrons. When such pairs enter the condensate they are converted into an exciton supercurrent, in such a way that

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the electron-hole flow across the sample is conserved. The latter exciton channel is preferred with respect to charge transmission, even if ω is just slightly above the gap. Therefore, the additional resistance arises due to the competition of exciton and charge currents, reminiscent of the interplay between electric supercurrent and heat flow at the NS junction. The effect is smeared as an insulating overlayer is inserted at the interface, spoiling the transparency of the junction: in the tunneling limit, exciton transport is suppressed. We further discuss physical systems which could show the effects our theory predicts.

The paper is organized as follows: In Section 2 we describe the solution of the electron transmission through the interface in terms of the two-band model of the SM/EI junction and in Section 3 we analyze the transport in terms of charge and exciton currents and examine the role of the exciton coherence. Then we study the interface differential conductance (Section 4), and lastly we review candidate experimental systems (Section 5).

2. Transport across the interface

We consider a junction made of a semimetal and an excitonic insulator. Specifically, the EI band structure originates from the renormalization of the SM energy bands, driven by Coulomb interaction. The EI gap corresponds to the binding energy of the electron–hole pairs which form a condensate. The interface discontinuity is solely brought about by the variation of the electron–hole pairing potential, $\Delta(z)$. This kind of junction could be experimentally realized by applying a pressure gradient or by inhomogeneously doping a sample grown by means of epitaxial techniques (see Section 5).

The electron and hole Fermi surfaces of the SM on the junction left-hand side are taken to be perfectly nested, the effective masses of the two bands being isotropic and equal to *m*. The quasi-particle excitations across the interface must satisfy the mean-field equations

$$\omega f(z) = -\frac{1}{2m} \left[\frac{\partial^2}{\partial z^2} + k_{\rm F}^2 \right] f(z) + \Delta(z) g(z), \tag{1a}$$

$$\omega g(z) = \frac{1}{2m} \left[\frac{\partial^2}{\partial z^2} + k_F^2 \right] g(z) + \Delta(z) f(z), \tag{1b}$$

with $k_{\rm F}$ Fermi wave vector and $\hbar=1$. The amplitudes f and g are the position-space representation of the electron quasiparticle across the interface: $|f|^2$ ($|g|^2$) is the probability for an electron of being in the conduction (valence) band, with energy $\omega > 0$ referenced from the chemical potential, which is in the middle of the EI gap due to symmetry. We assume Δ is a step function, $\Delta(z) = \Delta\theta(z)$.

In the elastic scattering process at the interface, all relevant quasi-particle states are those degenerate—with energy ω —on both sides of the junction. We handle the

interface by matching wave functions of the incident, transmitted, and reflected particles at the boundary. In the bulk EI, there are a pair of magnitudes of k associated with ω , namely

$$k^{+} = \sqrt{2m}\sqrt{k_{\rm F}^{2}/2m \pm (\omega^{2} - \Delta^{2})^{1/2}}.$$
 (2)

The total degeneracy of relevant states for each ω is fourfold: $\pm k^{\pm}$. The two states $\pm k^{+}$ have a dominant conduction-band character, while the two states $\pm k^{-}$ are mainly valence-band states. Using the notation

$$\Psi(z) = \begin{pmatrix} f(z) \\ g(z) \end{pmatrix} \tag{3}$$

the wave functions degenerate in ω are

$$\Psi_{\pm k^{+}} = \begin{pmatrix} u_0 \\ v_0 \end{pmatrix} e^{\pm ik^{+}z}, \quad \Psi_{\pm k^{-}} = \begin{pmatrix} v_0 \\ u_0 \end{pmatrix} e^{\pm ik^{-}z}, \tag{4}$$

with the amplitudes u_0 , v_0 defined as

$$u_0 = \sqrt{\frac{1}{2} \left[1 + \frac{(\omega^2 - \Delta^2)^{1/2}}{\omega} \right]},$$

$$v_0 = \sqrt{\frac{1}{2} \left[1 - \frac{(\omega^2 - \Delta^2)^{1/2}}{\omega} \right]},$$
(5)

possibly extended in the complex manifold. With regards to the SM bulk, $\Delta = 0$ and the two possible magnitudes of the momentum q reduce to $q^{\pm} = [2m(k_{\rm F}^2/2m \pm \omega)]^{1/2}$, with wave functions

$$\Psi_{\pm q^{+}} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{\pm iq^{+}z}, \quad \Psi_{\pm q^{-}} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} e^{\pm iq^{-}z},$$
 (6)

for conduction and valence bands, respectively.

The effect of an insulating layer or of localized disorder at the interface is modeled by a δ -function potential, namely $V(z) = H\delta(z)$ The appropriate boundary conditions, for particles traveling from SM to EI are as follows: (i) continuity of Ψ at z=0, so $\Psi_{\rm EI}(0) = \Psi_{\rm SM}(0) \equiv \Psi(0)$. (ii) $[f_{\rm EI}'(0) - f_{\rm SM}'(0)]/(2m) = Hf(0)$ and $[g_{\rm EI}'(0) - g_{\rm SM}'(0)]/(2m) = -Hg(0)$, the derivative boundary conditions appropriate for δ -functions [5]. (iii) Incoming (incident), reflected and transmitted wave directions are defined by their group velocities. We assume the incoming conduction band electron produces only outgoing particles, namely an electron incident from the left can only produce transmitted particles with positive group velocities $v_{\rm g} > 0$ and reflected ones with $v_{\rm g} < 0$.

Consider an electron incident on the interface from the SM with energy $\omega > \Delta$ and wave vector q^+ . There are four channels for outgoing particles, with probabilities A, B, C, D, and wave vectors $q^-, -q^+, k^+, -k^-$, respectively. In other words, C is the probability of transmission through the interface with a wave vector on the same (i.e., forward) side of its Fermi surface as q^+ (i.e., $q^+ \rightarrow k^+$, not $-k^-$), while

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