THEORETICAL STUDY OF QUANTUM SPIN/VALLEY HALL EFFECT IN BOROPHENE.

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Abstract

We study theoretically the quantum spin and quantum valley Hall effects in borophene. The particular emphasis is given to the effects of an electric field and intrinsic spin-orbit interaction. Strikingly, the tiltedness in the Dirac cone makes the electronic transport in borophene very different from other topological materials. Moreover, we investigate the effects of temperature on the electronic transport in borophene.

Introduction:

The study of 2D crystals and heterostructures has received great attention in the eld of nanoelectronics [1]. The successful synthesis of three dierent types of 2D crystalline boron structures has played an important role in this eld [2]. The 2D boron structure is known as borophene [3]. The theoretical study of borophene suggests that borophene exists in dierent allotropioc form [4]. It has been observed that Pmmn boron acts as Dirac semimetal, which has stable structure [4]. Furthermore, these Dirac semimetals have zero energy gap and satisfy low-energy electronic excitation law, called canonical dispersion law. The study of 2D and 3D Dirac semimetals and related materials like Weyl semimetals has played a signicant role in this research area. Initially graphene was discovered a 2D Dirac material, so it has been considered as main focus for the fundamental research with various potential applications. Nevertheless, the physics of Dirac semimetal Pmmn borophene is exciting as it shares some characteristics of graphene, while shows dissimilarities in other aspects, e.g, law of dispersion related to low energy excitation is anisotropic, contrary to graphene [4]. For the rst time it was considered that the crystal of borophene has tilted and anisotropic Dirac cone [4] which was proved experimentally later on [5].

In this research work, we are interested to study the eects of tiltedness in the Dirac cone on the electronic transport in borophene. We will extend the study to include the eects of applied homogenous electric eld and the spin-orbit interaction on the transport.

Model Hamiltonian:

The Hamiltonian for our system in cartesian coordinates reads [1]:

$$H = \zeta(v_x\sigma_x p_x + v_y\sigma_y p_y + v_t p_y) - \zeta s_z\, \boldsymbol{\Delta} so\,\sigma_z + \boldsymbol{\Delta}_z\sigma_z$$

$$E_{\boldsymbol{\lambda}}^{\zeta sz}(\tilde{p}) = \zeta v_e \tilde{p_y} + \lambda\sqrt{v_F^2\tilde{p}^2 + \boldsymbol{\Delta}^2}$$

Eigen Function

$$\psi(\lambda, k, s_z, \zeta) = \frac{1}{\sqrt{s}}\begin{pmatrix} cos\,\frac{\theta_\lambda^\zeta}{2} \\ sin\,\frac{\theta_\lambda^\zeta}{2}\,e^{\iota\Phi_k}\end{pmatrix} e^{\iota k.r}$$

Matrix Element of velocity operator.

$$v_x\zeta\zeta' = \zeta v_F\left[cos\frac{\theta_\lambda^\zeta}{2}\,sin\frac{\theta_{\lambda'}^\zeta}{2}\,e^{\iota\Phi_k} + cos\frac{\theta_{\lambda'}^\zeta}{2}\,sin\frac{\theta_\lambda^\zeta}{2}\,e^{-\iota\Phi_k}\right]$$

$$v_y\zeta\zeta' = -\iota\zeta v_F\left[cos\frac{\theta_\lambda^\zeta}{2}\,sin\frac{\theta_{\lambda'}^\zeta}{2}\,e^{\iota\Phi_k} - cos\frac{\theta_{\lambda'}^\zeta}{2}\,sin\frac{\theta_\lambda^\zeta}{2}\,e^{-\iota\Phi_k}\right] + \zeta v_e$$

Spsin and valley Hall conductivity

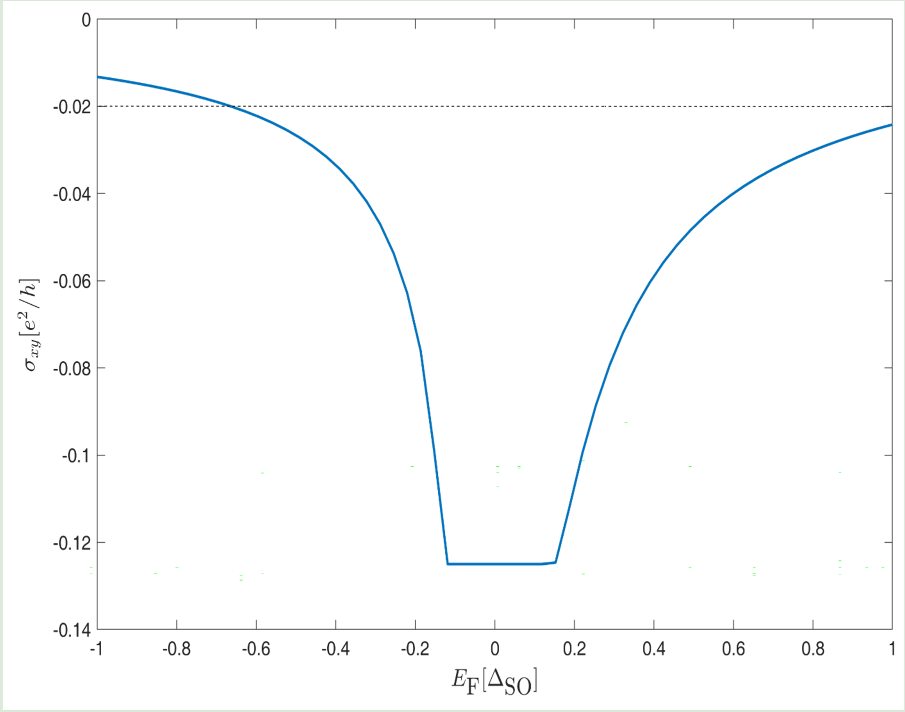
$$\sigma_{xy}(\zeta, s_z) = \frac{\iota\hbar e^2}{s}\sum\left[\frac{f\left(E_+^{\zeta,s_z}\right) - f\left(E_-^{\zeta,s_z}\right)}{\left(E_+^{\zeta,s_z} - E_-^{\zeta,s_z}\right)^2}\right]\times\left[\left\langle\psi_-^{\zeta,s_z}\middle|v_y\middle|\psi_+^{\zeta,s_z}\right\rangle\left\langle\psi_+^{\zeta,s_z}\middle|v_x\middle|\psi_-^{\zeta,s_z}\right\rangle\right]$$

$$\sigma_{xy}^v = \frac{e^2}{h}\left[\frac{\Delta_z - \Delta so}{\sqrt{(\Delta_z-\Delta so)^2 + \hbar^2 v^2 k_f^2}} + \frac{\Delta_z + \Delta so}{\sqrt{(\Delta_z-\Delta so)^2 + \hbar^2 v^2 k_f^2}}\right]$$

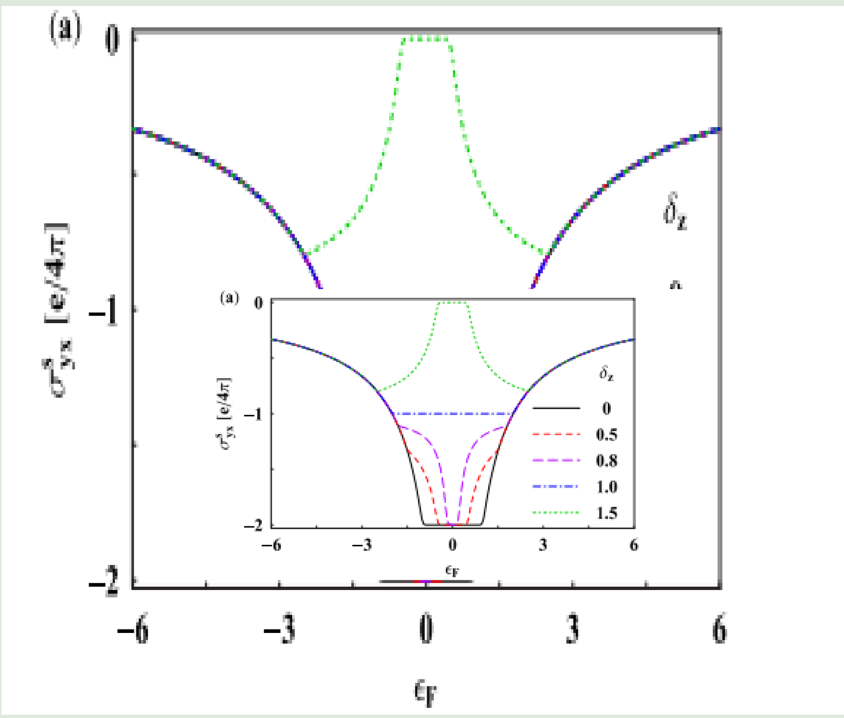
$$\sigma_{xy}^s = \frac{\hbar^2 e^2 v_f^2}{2(2\pi)^2}(\Delta_z - \Delta so)\int dk_x \int dk_y \frac{1}{[(\Delta_z-\Delta so)^2+\hbar^2 v^2 k_F^2]^{\frac{3}{2}}}\left[f(E_+^{--}) - f(E_-^{--}) - f(E_+^{++}) + f(E_-^{++})\right] + \frac{\hbar^2 e^2 v_f^2}{2(2\pi)^2}(\Delta_z + \Delta so)\int dk_x \int dk_y \frac{1}{[(\Delta_z-\Delta so)^2+\hbar^2 v^2 k_F^2]^{\frac{3}{2}}}\left[f(E_+^{+-}) - f(E_-^{+-}) - f(E_+^{-+}) + f(E_-^{-+})\right].$$

Numerical Simulations and Results:

Brophene



Silicene



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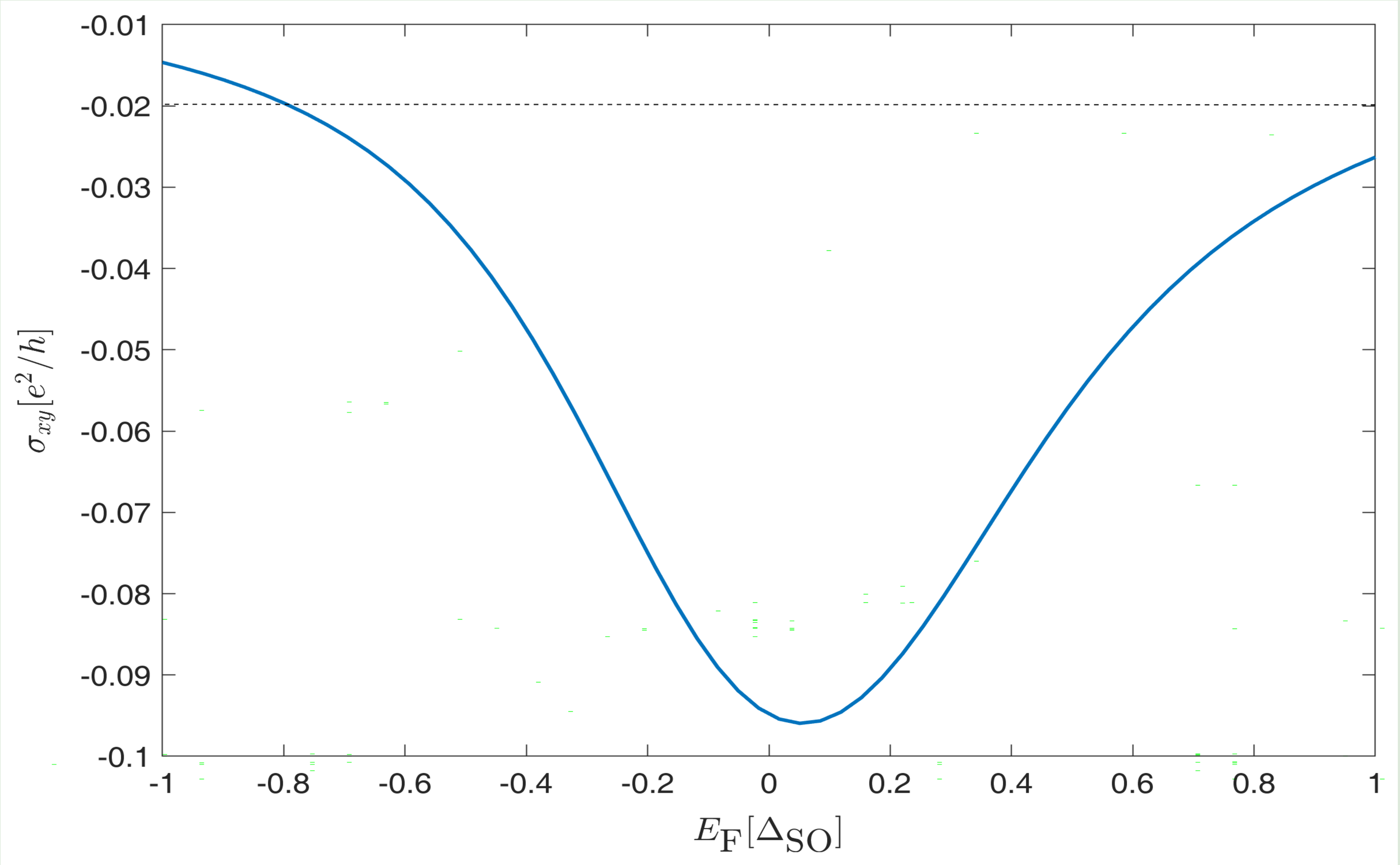

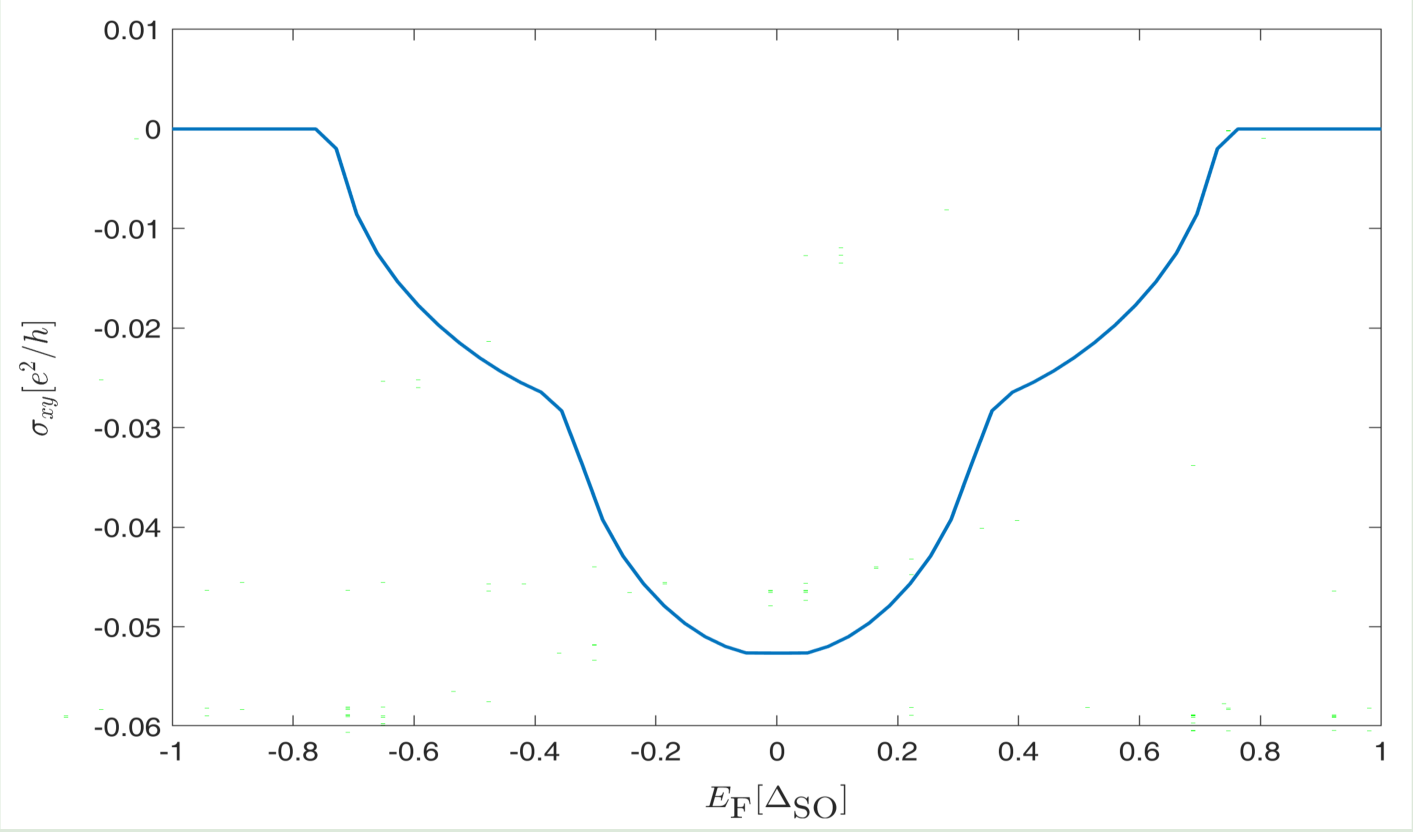

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