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Electronic heat capacity and magnetic susceptibility of ferromagnetic silicene sheet under strain

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ABSTRACT

The electronic heat capacity (EHC) and magnetic susceptibility (MS) of the two-dimensional material ferromagnetic graphene's silicon analog, silicene, are investigated by the strain-induced and the applied electric field within the Green's function technique and the Kane-Mele Hamiltonian. Dirac cone approximation has been performed to investigate the system under strain along the zigzag (ZZ) direction. The main attention is focused on the effects of external static electric field in the presence of strain on EHC and MS of a ferromagnetic silicene sheet. In the presence of strain, carriers have a larger effective mass and transport decreases. As a result, the temperature dependence of EHC and MS gives a critical strain around 10%. Furthermore, electric field breaks the reflection symmetry of the structure and a transition to the topological insulator for strained ferromagnetic silicene has occurred when the electric field is increased. In this phase, EHC and MS have weird behaviors with temperature.

1. Introduction

After the discovery of first real 2D-material graphene in 2004 [1], significant interest has been attracted in studying physical properties of 2D-materials both experimentally and theoretically with the honeycomb lattices such as hexagonal boron-nitride ($h-BN$), MoS_2 and recently a monolayer of silicon, known as silicene. Although these materials have a honeycomb lattice, but their properties are different [2–6]. In graphene, there is a minimal conductivity in the limit of zero doping, i.e., at Dirac points (K and K') which this can be understood because of its linear dispersion energy in the vicinity of K and K' valleys of the Brillouin zone [7,8]. This minimal conductivity creates a problem for using graphene as a highly motivated new material in electronic devices and electrical conduction can not be switched off by using the control voltages [9], which is essential for the operation of conventional transistors. One of the ways to overcome this problem is the creation of band gap in graphene electronic band structure which is made by inversion symmetry breaking [10,11]. It is desirable to have band gap in materials in addition to their novel features. Unlike graphene, according to the Fig. 1, silicene has a hexagonal atomic arrangement but due to its large ionic radius has a buckled configuration such that its sublattices (A and B) sit in two parallel planes with a vertical distance 0.46 nm [12–17]. The low-energy dynamics of fermions in graphene is described by the Dirac Hamiltonian for both valleys, but in silicene due to the strong spin-orbit (SO) interaction, carriers are massive with an energy gap around 1.55 meV [18,19]. This gap can be induced via an applied perpendicular electric field to its layer which leads to the many attractive properties of silicene [20–27]. The strain can change many features of 2D-materials. In graphene, Dirac points remain at K and K' points under biaxial strain, but they affected for strain along the different directions [28–31]. Contrary to the graphene, both the σ^* and π^* bands in silicene are more sensitive to the strain-induced [32–36]. For example, silicene becomes metallic under biaxial strain larger than 12% [32–34] and it turns into a metal under strain larger than 12% (14%) along the AC (ZZ) directions [36]. However, the investigation of thermodynamic properties of silicene under strain is still remain to be studied.

Unlike electronic properties, the thermal properties of silicence are still not well studied. Many works have been done in this case. For example, thermal conductivity of silicene is predicted around 20–65 W/mK [37–41]. The EHC of a semiconductor system is defined as the ratio of that portion of the heat used by the carriers (here, Dirac fermions) to the rise in temperature of the system. On the other hand, MS is the degree of magnetization of a material in response to an applied magnetic field. Our system is considered as ferromagnetic with an exchange field M. In this work, we have investigated the temperature dependence of EHC and MS in a ferromagnetic silicene sheet under strain at Dirac points., at a fixed strain modulus and direction of applied strain, EHC and MS are studied with electric field. Green's function approach is carried out within the Kane-Mele Hamiltonian. The outline of this paper is as follows: Section 2 describes the Hamiltonian and theoretical formalism. In Section 3, we show the

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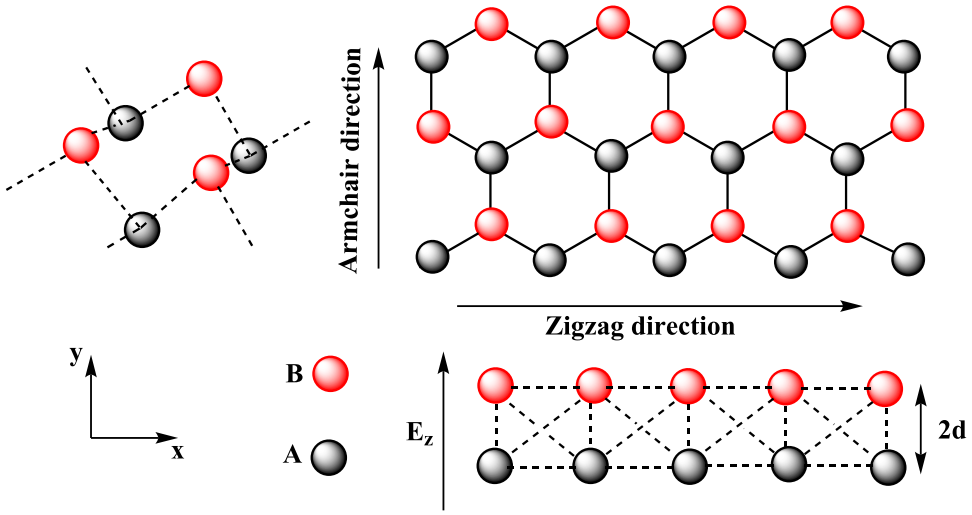

Fig. 1. Schematic illustration of silicene sheet. A and B sites separated by a distance $2d$ in the electric field E_z.

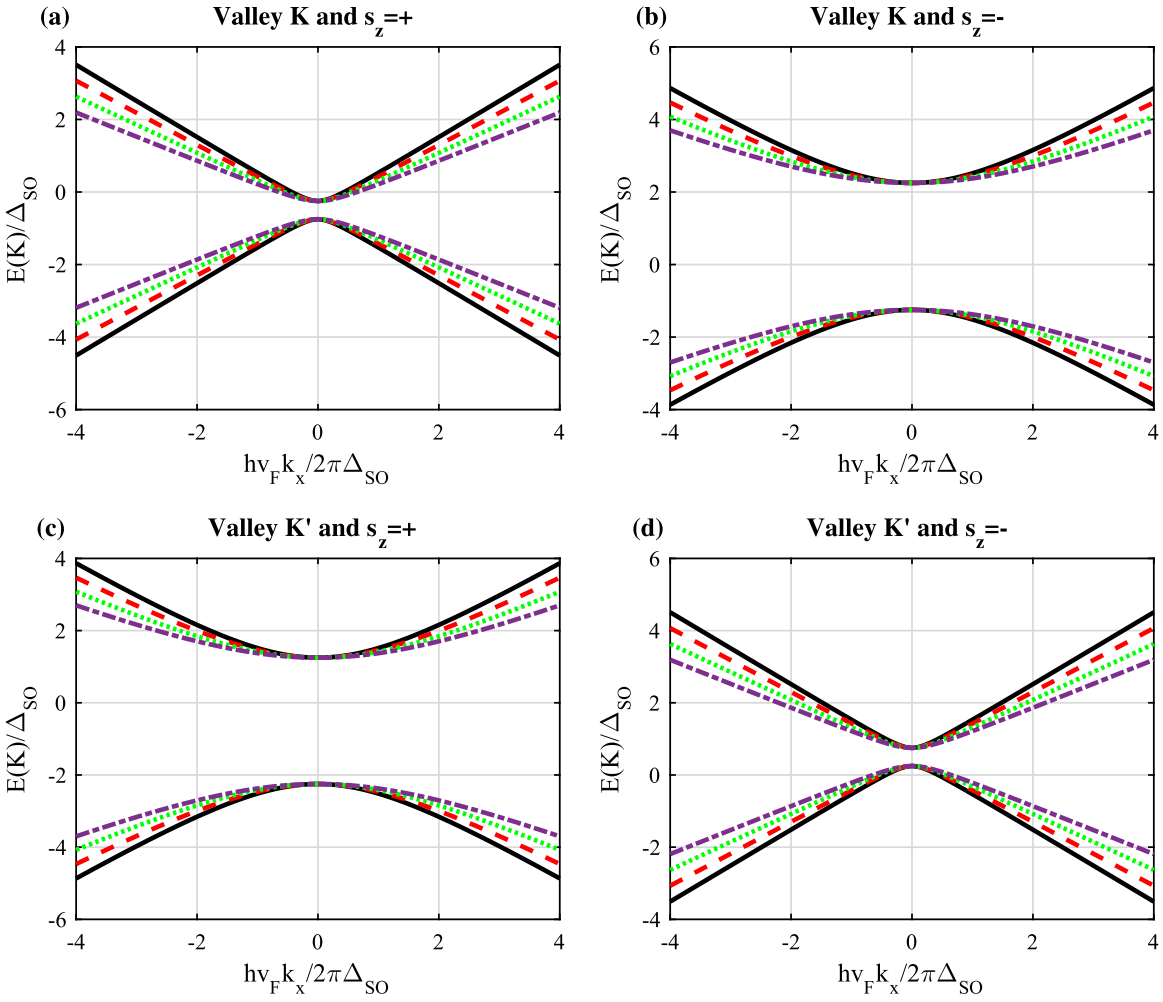

Fig. 2. (Colour online) The energy spectrum of ferromagnetic silicene with $M = \Delta_{SO}/2$ and $\Delta_z/\Delta_{SO} = 0.75$ for different strain modulus. $\epsilon = 0$ (black solid lines), $\epsilon = 5\%$ (red dashed lines), $\epsilon = 10\%$ (green dotted lines) and $\epsilon = 15\%$ (violet dotdashed lines).

EHC and MS of the system under strain and in Section 4, the numerical results are explained. Finally, Section 5 is the conclusion of the paper.

2. Theoretical formalism

In this section, we present the effective Hamiltonian model to describe the low-energy dynamics of carriers in a ferromagnetic silicene nanosheet which is subjected to a perpendicular uniform electric field as follows [18,42]

$$H_{\tau,s_z} = \hbar v_F (k_x \sigma_x - \tau k_y \sigma_y) - \tau s_z \Delta_{SO} \sigma_z + \Delta_z \sigma_z - M s_z \quad (1)$$

In our model, wave functions in the sublattice pseudospin space in