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A controllable magneto-topological property and band gap engineering in 2D ferromagnetic Lieb lattice

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Abstract

In this paper, we study theoretically the magneto-topological property and gap engineering of two-dimensional ferromagnetic Lieb lattice by taking into account the next-nearest-neighbors (NNN) coupling and the important Dzyaloshinsky-Moriya interaction (DMI). In particular, the density of states and dispersion energy of the system in terms of various NNN and DMI in the presence of Zeeman field produce the main features in the context of Heisenberg model, Holstein-Primakoff transformation, and Green's function approach. It is found that the inclusion of NNN coupling opens a gap, leading to the metal-semiconductor-insulator transition depending on its intensity. Furthermore, DMI introduces two extra degenerate bands in the vicinity of Fermi-level due to the Stark effect. The magneto-topological property of the gap in our model is determined by the tunneling probability of particles at both weak and strong NNN and DMI regimes. Finally, we discuss the extension of nuclear spins to arbitrary values.

Keywords: Lieb lattice, Green's function, Phase transition, Magneto-topological property, Nuclear spins

1. Introduction

A line-centered square depleted lattice, so-called two-dimensional (2D) Lieb lattice [1], is one of the interesting lattices with a novel flat band and infinite large effective mass [2, 3]. Interestingly, except designed artificial Lieb lattices, for instance, designing an artificial Lieb lattice on a metal surface by Wen-Xuan *et al.* [4], this lattice is existing in nature as high-temperature superconductor ($\text{La}_{2x}\text{Sr}_x\text{CuO}_4$ with the weakly coupled CuO_2 planes [5, 6]) with topological states [7, 8, 9, 10, 11, 12, 13]. The topology dependence of electronic properties of Lieb lattice has actuated researchers to find the fascinating properties originating from quantum fluctuations [14]. On the other hand, quantum effects in low dimensional spin systems have also been studied extensively over the past decade both theoretically and experimentally [15, 16, 17]. These systems opened new applications in real materials, for instance, in building

blocks in three dimensional perovskite materials [18] and photonic field [19, 20, 21, 22].

Motivated by the recent spintronic community, electric manipulation of the spin in Lieb lattice should also be possible and they can, therefore, be of value in real spintronics applications. The lattice has three sites A, B, and C per unit cell, as illustrated in the Fig. 1(a). The reciprocal lattice of this structure is also a square lattice [see Fig. 1(b)] with wave-vector coordinated $|\mathbf{K}| = \pi/a_0$ ($a_0 \simeq 0.95$ nm denotes the intra-atomic distance between A and B/C subsites) [5, 6, 8]. On the other hand, the one-particle energy spectrum of Lieb lattice in the absence of magnetic field, NNN, and DMI shows a three-band structure with electron-hole symmetry [23, 24], as shown in Fig. 1(c). One of the bands being flat and macroscopically degenerate (the middle one at $\mathcal{E}/J_1 = 0$). It has been shown that for the infinite Lieb lattice, the three energy bands touch each other in the middle of the spectrum (taken as the zero energy), and the low energy spectrum exhibits a Dirac cone located at the point $\Gamma = (\pi, \pi)$ in the first Brillouin zone (FBZ) as honeycomb lattice [25, 26].

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