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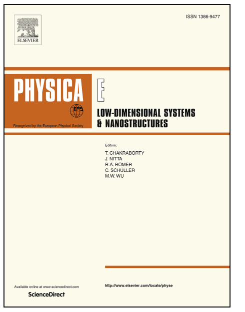

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Impurity-tuning of phase transition and mid-state in 2D spin Lieb lattice

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The bosonic phase of the three-band [one flat band and two dispersive bands] Lieb lattice can be significantly influenced by the impurity. Taking into account the combined Zeeman magnetic field, the next-nearest-neighbor (NNN) coupling, and the Dzyaloshinsky-Moriya interaction (DMI), we demonstrate this by studying the Heisenberg model on the spin $S = 1/2$ Lieb lattice. We perform numerical calculations of the density of states (DOS) within the Green's function method and the full-consistent Born approximation. The flat band becomes unstable upon the inclusion of the impurity and new degenerate- and mid-states appear. Our numerical results show that the energy of these states depends strongly on the NNN coupling, DMI, and the Zeeman splitting effect. Furthermore, we found different phase transitions, depending on the strengths of potentials above. Also, the number of van Hove singularities provided by DOS have a high susceptibility to the Hamiltonian model terms, which provides an intriguing possibility to control the finite impurity doping.

Key words: Lieb lattice, Green's function, Bosonic phase transition, Charged impurity, Born approximation

I. INTRODUCTION

The essential relation of two-dimensional (2D) lattices with flat energy bands to many-body effects have attracted great scientific interest for a half century [1–3]. One of the notable simplest 2D flat band systems is the Lieb lattice [4], which resembles the line-centered square depleted lattice [5–7]. This decorated lattice reported experimentally in various real materials such as $La_4Ba_2Cu_2O_{10}$ [8], $LaCo_5$ and $CePt_5$ [9]. Inherent evacuated sites in this lattice lead to one completely flat band and two dispersive bands with a mirror symmetry with respect to the flat band. Practically, these findings have been studied both theoretically and experimentally in Refs. [10–14]. These systems opened new applications in real materials, for instance, in building blocks in three-dimensional perovskite materials [15] and photonic field [16–19].

From these points, the eigenfunctions belonging to the Lieb lattice, for the flat bands, are entirely degenerate states, resulting in the infinite van Hove singularities in the non-interacting DOS. Impressing these flat bands leads to different physical properties of the system [20–22]. Furthermore, the effect of flat bands on the magnetic ordering states and electronic conventional and unconventional phases of different systems has been widely investigated [23–28]. Moreover, these flat bands support the induced topological phases [29–32]. Also, the effect of external electronic and magnetic perturbations on the variability of these flat bands has been studied in Refs. [33–38].

Recently, motivated by the spintronic community, electric manipulation of the spin Lieb lattice is valuable in real applications. To this end, 2D Lieb lattices have been experimentally realized in waveguide arrays [19, 39, 40], ultracold atoms in optical lattices [11, 13, 41], and also electronically [42, 43]. As mentioned, the flat bands in the Lieb lattices are extremely altered in the presence of external factors. Impurity doping as an external perturbation is one of the ways to tune the physical properties of a system. Since this type of perturbation affects and/or distributes the states of the particles, different bands and DOS are expected. Since all three bands show up the main features of the Lieb lattices, to the best of our knowledge, yet, the effect of impurities [in our case, dilute] on the phase of the Lieb lattice has not been studied theoretically well.

In the present paper, we study the dilute impurity effects on the phase of the spin Lieb lattice. We have employed the Heisenberg model and the Holstein-Primakoff transformation to describe the dynamics of non-interacting spin and eventually bosons. Then, we introduce the boson-impurity interaction using the Green's function approach within the full consistent Born approximation and T-matrix. Furthermore, in order to study the variation in the state ordering of the subsites, we consider the Zeeman magnetic field effect, which states that there is a coupling between external magnetic field and spins, combined by the NNN coupling and DMI fac-

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