Flat-band excitonic states in Kagome lattice on semiconductor surfaces

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1 Introduction

Recent surface techniques to fabricate and arrange quantum wires on the semiconductor surface have enabled to synthesize the artificial two-dimensional lattice systems such as square and triangle lattices. For example, C. Albrecht et al. produced a square lattice by arranging InAs wires on GaInAs (001) surface and showed that a butterfly energy spectra is seen in the case of applying the magnetic field. [1] Among various lattices, a Kagome lattice is located at the special position because of the appearance of complete flat bands in the electronic spectra. [2,3] Since the density of states of such flat bands is macroscopically large and the electronic correlation remarkably works when the half of a flat band is occupied by electrons through the application of the gate voltage, the surface ferromagnetism is predicted for nonmagnetic semiconductor surfaces [2,3] and the experimental challenges to realize a Kagome lattice is now in progress. In this view, one can also expect that a Kagome lattice shows an exotic optical properties, which have never been studied yet. In this paper, we investigated the excitonic properties of the Kagome lattice. Most remarkable finding is that the exciton binding energy on the Kagome lattice is extremely large; larger than that in one-dimensional system. Moreover, by calculating the binding energies of charged exciton and biexciton, we show that the excitons are easy to form charged exciton. We expect that the present results will give useful information for the optical detection of the flat bands.

2 Model and Method

The local spin density functional calculation showed that when quantum wires are arranged on the semiconductor surfaces in the way to form a Kagome lattice, the lower conduction-band electrons are mainly localized around the cross points of the quantum wires. [3] This enables us to reasonably assume that the electronic structures of electrons and holes in the lower conduction and higher valence bands are well described by employing the tight-binding model, where electrons and holes are located on the cross points of quantum wires and transfer along the wires. This situation is schematically shown as solid lines in Fig.1(b). Then the model Hamiltonian becomes

$$H = -\sum_{m,n} t_{mn} \hat{a}_{m}^{\dagger} \hat{a}_{n} - \sum_{m,n} t_{mn}^{b} \hat{b}_{m}^{\dagger} \hat{b}_{n} - \sum_{m,n} U_{mn}^{ab} \hat{a}_{m}^{\dagger} \hat{a}_{m} \hat{b}_{n}^{\dagger} \hat{b}_{n} ,$$

where $\hat{a}_{n}$ and $\hat{b}_{n}$ represent the annihilation operators of an electron and a hole at the $n$ site, respectively, and $t_{mn}^{a}$ and $t_{mn}^{b}$ are transfer energies of these carriers from the $n$ site to the $m$ site. $U_{mn}^{ab}$ is the Coulomb attraction energy between an electron and a hole, for which we adopted the following form;
\[ U^\text{ab}_{mn} = \begin{cases} U_0 & r = 0 \\ U_1/r & r \neq 0 \end{cases} , \]

where \( r_{mn} \) is the distance between \( m \) and \( n \) sites. [4] Here we assumed that the lattice constant is unity. The employment of this form of Coulomb energy is equivalent to the introduction of the cut-off parameter in one-dimensional systems to avoid the divergence and corresponds to the screening around the on-site. [4] The excitonic states are obtained as the lowest-energy bound eigenstates of this Hamiltonian. The exciton binding energy is calculated as the difference of energy between the lowest energy states with and without the Coulomb energy. The Hamiltonian is numerically diagonalized by the Lanczos method for Kagome lattice of the finite size as large as \( 18 \times 18 \). Since we are interested in qualitative features of excitons, in the calculation, the parameters are chosen adequately as \( U_0=0.1, U_1=0.75U_0 \), and \( t^a_{mn} = t^b_{mn} = -1.0 \). [4]

3 Calcuclated results and Discussions

3.1 Binding energy of exciton

First, we consider the exciton binding energy on the Kagome lattice. In order to characterize the Kagome system, we compare binding energies among various lattices. Two-dimensional Kagome, square, and triangle lattices and one-dimensional one are shown in Figs.1(a) to 1(c) as solid lines, respectively. It should be noticed here that, by introducing transfer energies, \( t' \), along broken lines in Figs.1(b) and 1(c) and gradually changing their values from \( t' = 0 \) to \( t' = -1 \), one can obtain Kagome and triangle lattices from one-dimensional and Kagome ones, respectively. This treatment enables us to study the effect of the continuous dimension reduction of a lattice on the exciton binding energy from two to one by way of a Kagome lattice. In the followings, we also consider these lattice systems between triangle and one-dimensional lattices with varying the transfer energies, \( t' \).

Figure 1: The lattice models adopted in this work: (a) triangle, (b) Kagome, (c) one-dimensional, and (d) square lattices are shown by solid lines. Kagome and one-dimensional lattices are obtained from triangle and Kagome ones, respectively, by removing transfer energies shown by broken lines in (b) and (c).

Figure 2 shows the calculated binding energies of exciton for various lattices. It is well known that the exciton binding energy becomes large as the dimensionality of the system decreases. As expected from this result, the binding energies in two-dimensional triangle and square lattices are smaller than one-dimensional lattice. However, in spite that the bond connection decreases in a one-dimensional lattice compared to a Kagome one, the exciton binding energy in the Kagome lattice is much larger than the one-dimensional one. To clarify the excitonic feature furthermore, the calculated exciton wave functions are shown in Fig.3 for Kagome, one-dimensional, and triangle lattices. This figure represents the spatial distribution of a hole as a function of the distance, \( r \), between a hole and an electron when the electron is fixed on the \( r=0 \) site, where the distance, \( r \), is measured in units of lattice constant and taken along one direction. As seen in Fig.3 the excitonic radius is extremely small, around two lattice sites, in the Kagome lattice, being much smaller than the other lattices discussed in this paper. Apparently, these results reflect the localized nature of flat-band states, i.e. the conduction-band electron and valence-band
hole states in the Kagome lattice.

Next, we consider the variation of exciton binding energy when the magnetic field is applied perpendicular to the surface. In the tight-binding model, the magnetic field effect is introduced into the Hamiltonian by multiplying the transfer energy $t_{mn}$ by the phase factor, $\exp\left[i\frac{2\pi e}{\hbar c} \int_A \mathbf{A} \cdot dr\right]$, where $\mathbf{A}$ is the vector potential. In the case of no Coulomb interaction, with increasing the magnetic field, the flat band becomes dispersive and its position leaves from the conduction-band bottom to the conduction-band top, which also applies to the valence band. Figure 4 shows the calculated exciton binding energy as a function of magnetic field, where the magnetic field corresponds to the flux in the unit cell of Kagome lattice and is measured in the unit of flux quantum. In insert, we also display the schematic band dispersion of the conduction band in the cases of zero and one flux quantum. It is seen that the exciton binding energy is the largest in the case of no magnetic field and suddenly decreases with applying the magnetic field. This indicates that one can largely control the binding energy of excitation by using a Kagome lattice, and the flatness of the lowest-conduction and highest-valence bands is essential to the large exciton binding energy. Moreover, we note that the binding energy with magnetic field shows complicated variation and changes between those of one and two-dimensional lattices, the reason of which has not been clarified yet.

3.2 Stability of exciton

Then we consider the stability of excitonic state. Since the radius of flat-band exciton is extremely small as shown above, the high exciton density is expected when the system is highly excited. Thus, we consider the stability of exciton by calculating the binding energies of charged exciton and biexciton, which are made of two electrons and one hole, and two electrons and two holes, respectively. The binding energies of these exciton complexes are calculated in a similar way to that of exciton, where the similar Coulomb repulsion interaction is introduced between electrons or holes. Moreover, we treat elec-
Figure 4: Calculated exciton binding energy as a function of magnetic field perpendicular to the Kagome lattice plane. Calculations are performed for $15 \times 15$ unit. Binding energies of two-dimensional (2-dim) triangle and one-dimensional (1-dim) lattices are denoted by arrows.

electrons and holes as spinless fermions, thus the exciton complexes corresponding to spin-singlet states. The calculated binding energies of the exciton, charged exciton and biexciton are shown in Fig.5. It is seen that the biexciton is unstable, while the charged exciton becomes stable. This might be related to the localized nature of carriers in a Kagome lattice. However, the detailed analysis is now processing and will be published elsewhere.

4 Conclusion

We have investigated the excitonic properties in Kagome lattice system by using the exact diagonalization of a tight binding model. The following features are clarified. (1) The exciton binding energy in the Kagome lattice is much larger than those in another two-dimensional systems, such as triangle and square lattices, and even the one-dimensional one. Furthermore the exciton radius is extremely small in the Kagome lattice, compared with the other lattices discussed in this paper. (2) The exciton binding energy is the largest in the case of no magnetic field, and suddenly decreases with applying the magnetic field. (3) When we treat electrons and holes as spinless

Figure 5: Calculated binding energies of 2, 3, and 4 particle states in the Kagome lattice. (a) States with one electron and one hole, (b) states with two electrons and one hole, and (c) states with two electrons and two holes. In (b), for examples, e-h,e schematically represents that one electron and one hole produce a bound state, while the other electron is not bounded. Calculations are performed for $3 \times 3$ unit.
fermions, the biexciton is unstable, while the charged exciton becomes stable.

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6 Reference

[1] C. Albrecht, J. H. Smet, K. von Klizing, D. Weiss, V. Umansky and H. Schweizer, Phys. Rev. Lett. 86, (2001) 147.

[2] A. Mielke and H. Tasaki, Commun. Math. Phys. 158, (1993) 341.

[3] K. Shiraishi, H. Tanura and H. Takayanagi, Appl. Phys. Lett. 78, (2001) 3702.

[4] K. Ishida, Phys. Rev. B. 49, (1994) 5541.