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Magnetic-field effects on a two-dimensional Kagomé lattice of quantum dots

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Magnetic-field effects on the energy spectrum (Hofstadter butterfly) and the flat-band ferromagnetism are studied on a two-dimensional Kagomé lattice of quantum dots. Application of a perpendicular magnetic field destroys the flat-band ferromagnetism and induces a metal-insulator transition because the flat band has a finite dispersion. In the half-filled flat band, the ferromagnetic-paramagnetic transition and the metal-insulator one occur simultaneously at a magnetic field when the Coulomb interaction is strong. These phenomena can be observed in experiment under reasonable magnetic fields in artificial quantum dot superlattices.

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Tailoring the band structure and electronic properties has been attempted since 1970s by stacking a sequence of semiconductors with different band gaps to produce new materials and devices called semiconductor superlattices. The energy spectrum of the vertical superlattice is determined by the artificial periodicity and the coupling between quantum wells rather than by the properties of the individual semiconductor materials. Recent progress in semiconductor nanofabrication technology provides us the route to realize an artificial crystal made of quantum dots located on sites of a lattice and coupled to each other, which is called a quantum dot superlattice (QDSL). In arbitrary lattice patterns, the period of the lattice and the coupling between dots can be adjusted to engineer the band structure. A recent experiment of the quantized Hall conductance of the two-dimensional electron gas (2DEG) in a periodic potential with square symmetry has provided evidence of minigaps in the energy spectrum (Hofstadter's butterfly)[1] induced by a perpendicular magnetic field. This experiment showed that a uniform artificial lattice can be fabricated with sufficient accuracy by existing technology. For further advance in nanotechnology, it is very important that we propose theoretical ideas for various lattice patterns with possible interesting effects, which might not be realized in real materials.

Recently, the present authors have proposed the idea of making the QDSL ferromagnetic on some bipartite lattices[2,3] and the Kagomé lattice structure[4] by existing technology without any magnetic element. This idea is based on the mathematical theorem, rigorously proven in a Hubbard model on bipartite lattices[5] and the Kagomé lattice[6], that the ground state is ferromagnetic at zero temperature on these lattices where the single-particle-energy spectra have dispersionless flat bands in the tight-binding approximation.[7] Several other proposals of ways to achieve the flat-band ferromagnetism in real materials have been made.[8–10] At present, however, there is no clear evidence of flat-band ferromagnetism in real materials, mainly because the electron filling is very hard to be controlled and the Jahn-Teller effect lifts the degeneracy of the flat band by the lattice distortion. In the QDSL, on the other hand, we can avoid such problems, and, moreover, various lattice patterns can be designed by a lithography technique. Therefore, the QDSL is quite suitable for observing the flat-band ferromagnetism. The QDSL also features tunable magnetic-field effects. In normal crystals the magnetic field needed to put a magnetic-flux quantum in a unit cell having a lattice constant of few angstroms is typically of the order of 10^4 T. But in the QDSL with a lattice constant of more than few ten nanometers, the magnetic field required is at most few tesla, which is reasonable and easily tunable.[11] Hence, the magnetic-field effects on the flat-band ferromagnetism are worth studying on the dot lattice.

In this paper, we study magnetic-field effects on the Kagomé QDSL. The magnetic field destroys the flat band and causes a finite dispersion in the energy spectrum because it disturbs the interference of the phases of wave functions. The flat-band ferromagnetism is also broken by the magnetic field, which can be understood in terms of the competition between the effective exchange energy and the single-particle energy. The breakdown of the flat band also causes a metal-insulator transition induced by the magnetic field. Furthermore, when the flat band is half-filled, the ferromagnetic-paramagnetic transition and the metal-insulator one occur simultaneously when the Coulomb interaction between electrons is strong.

Let us start by examining the single-particle property of the Kagomé lattice in a magnetic field. We assume a tight-binding model for the Kagomé lattice as illustrated in Fig. 1(a). The calculated band structure in zero magnetic field contains the flat band [Fig. 1(b)]. The magnetic flux is incorporated in hopping integral t_{ij} through the Peierls phase for a gauge field as

$$t_{ij}(\mathbf{A}) \equiv t\exp(i\theta_{ij}), \quad \theta_{ij} = -\frac{2\pi}{\phi_0}\int_{\mathbf{r}_i}^{\mathbf{r}_j} \mathbf{A}\cdot d\mathbf{r}, \tag{1}$$

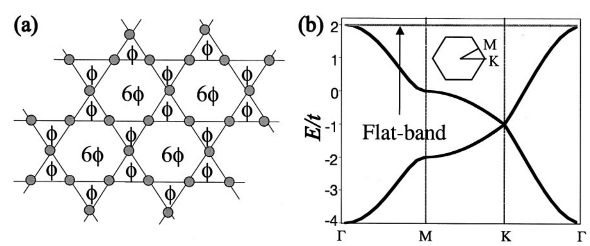

FIG. 1. The Kagomé lattice structure (a) and the band structure of the tight-binding model at zero magnetic field (b). The magnetic flux through the Kagomé lattice is also shown in (a).

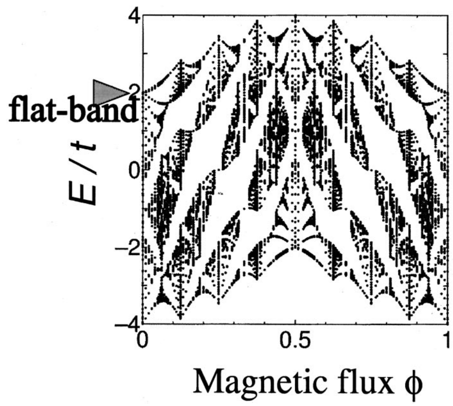

FIG. 2. The single-particle energy spectrum in the magnetic field (i.e., Hofstadter's butterfly). The arrow points to the position of the flat band ($E/t=2$) in zero magnetic field.

where **A** is the vector potential of the magnetic field threaded perpendicularly to the 2D plane, $\phi_0 \equiv h/e \equiv 1$ is the magnetic-flux quantum through the smallest triangle in a unit cell, and $t(>0)$ is the hopping integral at zero magnetic field. Hereafter, we define ϕ as the magnetic flux through the smallest triangle in a unit cell [Fig. 1(a)]. Calculated results for the Hofstadter butterfly (the single-particle energy spectrum) of the Kagomé lattice are shown in Fig. 2. Note that the flat band at the $E/t=2$ in zero magnetic field is broken by applying the magnetic field. In the Kagomé lattice, the magnetic field affects the interference between the electron wave functions.[12] As a result, the magnetic field breaks the interference-originated flat band in the Kagomé lattice.[13] For $\phi = n/8m$ (n, m: integer), there are $3m$ magnetic minibands, and for $\phi = n/8$ the number of the magnetic minibands is smallest and the band gap is widest. In real systems, it is indeed difficult to observe the small band-gap structures of the Hofstadter butterfly because they are easily smeared out by an inevitable decoherence of the wave functions. Hence, large band-gap structures, such as at $\phi = n/8$, will be experimentally relevant.

We have to include the Coulomb interaction between electrons in order to study the flat-band ferromagnetism in the magnetic field. Let us assume the Hubbard model with the on-site interaction U between electrons with opposite spins. The Hamiltonian of the Hubbard model is written as

$$H = -\sum_{\langle i,j\rangle,\sigma} [t_{ij}(\mathbf{A}) c^{\dagger}_{i\sigma} c_{j\sigma} + \text{H.c.}] + U \sum_i n_{i\uparrow} n_{i\downarrow}, \quad (2)$$

where $n_{i\sigma} \equiv c^{\dagger}_{i\sigma} c_{i\sigma}$, $c_{i\sigma}$ annihilates an electron with spin σ at site i, and $\langle \cdots \rangle$ refers to pairs of nearest neighbors. In our numerical calculation, we perform an exact diagonalization of a finite-size cluster of the Hubbard model on the Kagomé lattice with the Lanzos algorithm. This method has been used in Ref. 14 to study the flat-band ferromagnetism at zero magnetic field and it has been verified that the numerical results are fully consistent with Mielke's theorem for proving the ferromagnetism on the Kagomé lattice having infinite lattice points.[6] We employed the antiperiodic boundary condition to avoid excess degeneracy at the Γ point [see Fig. 1(b)] to reduce the finite-size effects. Calculated results for the magnetic-field dependence on the flat-band ferromagnetism of the 12-site (2×2 unit cells) cluster are shown in Table I, where the total spins of the ground states are presented for the filling that equals ($N=20$) or is slightly larger ($N=21$) than half-filling where Mielke's proof can be applied for the flat-band ferromagnetism at zero magnetic field. We can see the ferromagnetic-paramagnetic transition induced by the magnetic field. The high-spin state at zero magnetic field originates from an effective exchange interaction with strength of the order of $-t$,[15] which always makes spins align when electrons are in the energetically degenerate flat band.[16] Once the flat band is broken and the degeneracy is lifted by the magnetic field, the gain in the single-particle energy of the low-spin states can overcome that of the exchange energy in the high-spin state and the flat-band ferromagnetism disappears.[17] This ferromagnetic-paramagnetic transition is an unusual type of magnetic-field effect and seems counter-intuitive because the magnetic field usually supports ferromagnetism by Zeeman coupling, which favors the aligned spins along the direction of the magnetic field. Here, we note that the results for a larger cluster of 3×2 unit cells are qualitatively the same as those for 2×2 unit cells.

TABLE I. Total spins of the ground state of the 12-site (2×2 unit cells) Kagomé Hubbard cluster with $U/t=5$ are shown as a function of the electron number N and magnetic flux ϕ.

	ϕ				
N	0	1/8	1/4	3/8	1/2
20	2	2	0	0	0
21	3/2	3/2	1/2	1/2	1/2

The magnetic-field effect on the energy spectrum and the ground-state properties discussed so far also reflect the transport properties of the QDSL. We discuss the magnetoresistance when the flat band crosses the Fermi level. We calculate the Drude weight D, which is defined as the zero frequency part of the optical conductivity $\sigma(\omega) \equiv D\delta(\omega)$ +(regular part for finite ω). The Drude weight is given by[18]

$$\frac{D}{2\pi e^2} = -\frac{\langle \Psi_0 | \hat{K} | \Psi_0 \rangle}{2N_s} - \frac{1}{N_s} \sum_{n\neq 0} \frac{|\langle \Psi_n | \hat{J} | \Psi_0 \rangle|^2}{E_n - E_0}. \quad (3)$$

Here $\Psi_{0(n)}$ is the ground (nth excited) state with an energy eigenvalue $E_{0(n)}$, N_s is the number of sites, $\hat{J}$ is the current operator, and $\hat{K}$ is the ''kinetic energy'' operator along the direction of the current. In the bulk limit $N_s \to \infty$, generally speaking; $D=0$ means that the system is insulating, while $D>0$ means it is metallic (or superconducting). Figure 3 shows the magnetic-field dependence of the Drude weight of the ground states for Kagomé clusters with 2×2 unit cells.[19] The calculated Drude weights for 3×2 unit cells are again qualitatively the same as those for 2×2 unit cells. Let us look at the case when the filling is away from half-filled on the flat band. All the data of the Drude weight are overlapped at $D=0$ at zero magnetic field, indicating an insulating behavior, and become finite when the magnetic field is applied,

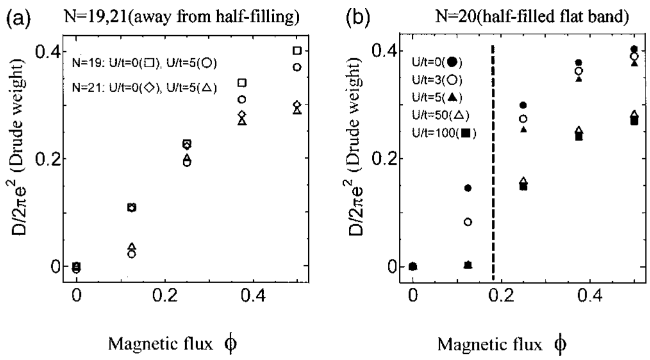

FIG. 3. Magnetic-field dependence of the Drude weights of a 12-site (2×2 unit cells) Kagomé Hubbard cluster is shown. (a) shows the results when the filling is away from half-filling of the flat band with $U/t=0$ (squares for $N=19$ and diamonds for $N=21$) and $U/t=5$ (circles for $N=19$ and triangles for $N=21$). (b) shows the results at half-filling ($N=20$) with $U/t=0$ (filled circles), 3 (open circles), 5 (filled triangles), 50 (open triangles), and 100 (filled squares). The vertical dashed line separates the ferromagnetic and insulating region (left side) and the paramagnetic and metallic region (right side) for $U/t=5,50,100$.

indicating a metallic behavior [Fig. 3(a)]. The metal-insulator transition induced by the magnetic field will manifest itself in the giant negative magnetoresistance of the Kagomé QDSL. This phenomenon can be clearly understood in terms of a single-particle picture. The group velocity of electrons is zero without the magnetic field and the system is insulating. In the presence of the magnetic field ($0<\phi\leqslant0.5$), the flat band has a finite curvature and the group velocity becomes finite, resulting in the metallic behavior.

Next, we calculate the Drude weights at the half-filled flat band [Fig. 3(b)]. For small $U/t<3.8$ [represented by data for $U/t=0,3$ in Fig. 3(b)], the insulating system turns metallic by applying the magnetic field, which is qualitatively the same behavior as that for the case away from half-filling. However, for large U/t [represented by data for $U/t=5,50,100$ in Fig. 3(b)], the high-spin ($S=2$) states have negligible Drude weights at $\phi=1/8$ (where the data for $U/t=5,50,100$ are almost completely overlapped at $D\simeq0$) and they turn into low-spin ($S=0$) and metallic states with finite Drude weights above $\phi=1/4$. The physical picture of this simultaneous transition between the metallic-insulating and the ferromagnetic-paramagnetic states at the magnetic field from $\phi=1/8$ to 1/4 is as follows. When the ground state is ferromagnetic for a large U below $\phi=1/8$, all up-spin states on the (nearly) flat band are completely occupied at half-filling, while all down-spin states are unoccupied. In the absence of spin-flipping processes like in the present case, up-spin electrons on the flat band cannot transit in the k space because of Pauli's exclusion principle, which results in the insulating state at half-filling at $\phi=1/8$. Above $\phi=1/4$, the ground states come to have a low spin value where both unoccupied and occupied states coexist in both up- and down-spin states and electrons can now move, resulting the metallic behavior. Here, we make one remark: the Drude weight seems to converge to a finite value for the large U/t limit for low-spin states.[20] This eliminates the possibility of the Mott transition in low-spin states which occurs in single-band Hubbard models at half-filling, where the electron number per one site is exactly one and the interaction energy (of the order of U) is needed for one electron to move from one site to its nearest neighbor. In the Kagomé lattice, on the other hand, the electron number chosen in Fig. 3 is not half-filling in the real space even though the flat band is half-filled.

Finally, we discuss the experimental relevance of the present results. As an example, we discuss the InAs Kagomé QDSL proposed in Ref. 4, which has a dot-diameter of about 200 nm and a lattice constant of 720 nm. The hopping integral t is evaluated as 1.5 meV from the bandwidth and the on-site Coulomb energy U is estimated as 30 meV from the size of dot. The largest gaps at $\phi=1/8$ in the Hofstadter's butterfly shown in Fig. 2 are roughly estimated as $t\sim1.5$ meV. To detect these gaps in real experiments, this energy gap (or the hopping parameter) should be larger than the temperature and the broadening caused by imperfections and disorder. The Zeeman effect can be negligible in a QDSL. In the present example, the magnetic field needed to put a magnetic-flux quantum into the smallest triangle of the Kagomé lattice having the lattice constant of 720 nm is about 0.07 T, which corresponds to the Zeeman coupling ~0.03 meV, which is much smaller than the hopping integral $t\sim1.5$ meV. The coupling between the magnetic field and orbital angular momentum would probably be small due to the s-wave-like nature of the lowest state in the quantum dot as demonstrated in Ref. 4.

In conclusion, we have studied magnetic-field effects on a 2D Kagomé lattice. The energy spectrum is obtained as a function of the magnetic flux and the flat band is destroyed at finite magnetic flux. The ferromagnetic-paramagnetic and metal-insulator transitions induced by the magnetic field are predicted. For the half-filled flat band, we find that the metal-insulator transition occurs simultaneously with the ferromagnetic-paramagnetic one for large U/t at a magnetic field. These magnetic-field effects should be observable for reasonable (order of 0.1T) magnetic fields in the QDSL in a controllable way by existing technology.

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[19] Exactly speaking, the Drude weight slightly depends on the direction of the current not qualitatively but quantitatively. We present only the Drude weights for the direction that is perpendicular to a side of the smallest triangle in the unit cell.

[20] We indeed find that a high-spin ground state appears again for very large $U/t\geqslant111$ at $\phi=1/4$. However, we doubt whether such a transition at the very large value of U/t can be considered realistic, because it may due to a finite-size effect. A more reliable analysis of this problem remains as a future work.