Magnetic field effects on two-dimensional Kagome lattices

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Abstract

Magnetic field effects on single-particle energy bands (Hofstadter butterfly), Hall conductance, flat-band ferromagnetism, and magnetoresistance of two-dimensional Kagome lattices are studied. The flat-band ferromagnetism is shown to be broken as the flat-band has finite dispersion in the magnetic field. A metal-insulator transition induced by the magnetic field (giant negative magnetoresistance) is predicted. In the half-filled flat band, the ferromagnetic-paramagnetic transition and the metal-insulator one occur simultaneously at a magnetic field for strongly interacting electrons. All of the important magnetic fields effects should be observable in mesoscopic systems such as quantum dot superlattices.

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For the last two decades, low-dimensional systems have been one of the most important subjects of research in condensed matter physics. Especially, two-dimensional (2D) electron systems have been of great interest because of striking phenomena such as high-Tc superconductivity, and the (fractional) quantum Hall effect (QHE). For the last decade, the ferromagnetism of 2D systems has also attracted attention, especially for systems without any magnetic elements. The ferromagnetism of the 2D electron gas has never been observed because the parameter, which is the ratio of the mean distance between nearest electrons to the Bohr radius, must become very large (∼40) for the ferromagnetism even if we neglect the Wigner crystallization. However, the ferromagnetism has been rigorously proved for Hubbard models on some lattice structures having a flat band (FB) \[2–4\]. The flat-band ferromagnetism (FBF) is not only expected as a starting point for understanding the ferromagnetism of itinerant electrons but also for fabrication to make a FB in real materials \[5–7\]. At present, however, there is no clear evidence of the FBF in real materials because of difficulties such as uncontrollable electron filling and the Jahn-Teller effect that breaks the FB degeneracy. Recently, we have proposed a method of making an effective Hubbard model with some bipartite lattices and the Kagome lattice structure \[8,9\], which have a FB, in mesoscopic quantum dot superlattices. For dot superlattices, we can avoid the above-mentioned problems in bulk systems, and the parameters of the Hubbard model, the electron filling, and the lattice structure can be freely changed. Furthermore, there is another important advantage of a mesoscopic system when we study magnetic field effects. Of course, there are lots of important magnetic field effects in bulk systems. However, in dot superlattices it is easy to study magnetic field effects at the lattice level, such as the Hofstadter butterfly and lattice QHE \[10\]. In bulk systems the magnetic field that is needed in order to input a magnetic-flux quantum within a unit cell, which has a lattice constant of few angstroms, is of the order of \(10^4\) T, but in dot superlattices, the magnetic field needed is very small and realistic. For example, in Kagome dot superlattices proposed in Ref. \[9\], the lattice constant is of the order of 100 nm, and the magnetic field needed is of the order of 0.1 T. In addition, if we pay attention to the many-body effects of electrons, it is quite interesting to study the magnetic field effects on the FBF of the Kagome lattice.

In this Letter, we study magnetic field effects on the Kagome lattice. In the magnetic field, the FB is broken down because it originates from the interference of the phases of wave functions. Hall conductance at a magnetic field is shown to have a wide Hall plateau, which may be easily observable in experiments. The FBF, which has been mathematically proved by Mielke \[3\], is also broken by the magnetic field, which is understood to be a result of competition between generalized Hund’s coupling and the single-particle energy. This ferromagnetic-paramagnetic transition is a new magnetic field effect. Usually, the magnetic field supports ferromagnetism by Zeeman coupling, which favors the aligned spins along the direction of the magnetic field. We should note that in dot superlattices the Zeeman effects are negligible for small magnetic field. We also find a giant negative magnetoresistance (GNMR), which is the metal-insulator transition induced by the magnetic field that breaks the FB. Furthermore, when the FB is half-filled, the ferromagnetic-paramagnetic transition and the metal-insulator one occur simultaneously for strongly interacting electrons in a magnetic field.

Let us start from the single-particle properties of the Kagome lattice in a magnetic field. We assume a tight-binding model for the Kagome lattice [Fig. 1(a)]. The magnetic field
is incorporated in hopping integral $t_{ij}$ in the usual manner through the Peierls phase for a
gauge field as

$$t_{ij}(A) \equiv t \exp(i\theta_{ij}), \quad \theta_{ij} = -\frac{2\pi}{\phi_0} \int_{r_i}^{r_j} A \cdot dr,$$

(1)

where $A$ is a vector potential for the magnetic field $\phi$, $\phi_0 \equiv h/e$ is the magnetic-flux quantum,
and $t(>0)$ is the hopping integral at zero magnetic field. Hereafter, we use a unit where
a magnetic-flux quantum through the smallest triangle in a unit cell is defined as unity.
Our result for the Hofstadter butterfly (the single-particle energy spectrum) of the Kagome
lattice is shown in Fig 1(b). When there is no magnetic field, there is a FB at the $E/t = 2$
[Fig. (2)] and it is broken by applying magnetic field. The magnetic field changes the phase
of the wave function and the interference between the electron wave functions. As a result,
the magnetic field breaks the interference-originated FB in the Kagome lattice. We note that
the FB is not always broken by a magnetic field for other lattice structures. For example,
the FB of the Lieb lattice is preserved even in a magnetic field [11]. The difference is due to
the origins of the FBs. In the Lieb lattice the FB originates not from the interference but
from the lattice topology. Let us revert to the subject of the Kagome lattice. In the Kagome
lattice, for $\phi = n/8m$ ($n$, $m$: integer), there are $3m$ magnetic bands, and for $\phi = n/8$ the
number of the magnetic bands is smallest and the band gap is widest. In real systems it
is indeed difficult to observe the physical properties of the small band-gap structures of the
Hofstadter butterfly because of the inevitable decoherence of the wave functions. Hence
only the large band-gap structures, such as $\phi = n/8$, will be experimentally important. On
the other hand, it is well known that the quantized Hall conductance reflects the band-gap
structures directly. We calculated the Hall conductance, which is equivalent to the Hall
conductivity in 2D, with the Kubo formula [12,13]. Figure 3 shows the Hall conductance as
a function of Fermi energy for $\phi = 1/8$ and $1/4$. Especially for $\phi = 1/4$, we can see a wide
quantized Hall plateau reflecting a wide band gap: there is indeed a flat band at $E/t = 0$,
but its contribution to the conductance is zero and the plateau is not changed there. The
QHE may be observable in experiments without great effort because of the wide plateau.
We neglected the interaction between electrons in the above calculations. But if we assume
the interaction is not so strong and short-ranged, such as that in quantum dot superlattices,
it may not significantly affect the Hall plateau.

We must consider the interaction between electrons to study the FBF. Let us consider
the Hubbard model with the on-site interaction $U$ between electrons with opposite spins.
The Hamiltonian is written as

$$H = -\sum_{<i,j>} (t_{ij}(A)c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow},$$

(2)

where $n_{i\sigma} \equiv c_{i\sigma}^\dagger c_{i\sigma}$, $c_{i\sigma}$ annihilates an electron with spin $\sigma$ at site $i$, and $< \ldots >$ refers
to pairs of nearest neighbors. For the Kagome Hubbard lattice without a magnetic field,
Mielke [3] has mathematically proved the ferromagnetic behavior in a finite region where the
filling of the FB equals or is slightly larger than the half-filling. Reference [14] has studied
the Kagome Hubbard cluster without a magnetic field. There we can see the highest-spin
state for the half-filled FB, and the height of the total spin is gradually decreased for larger
filings as expected.
We study the magnetic field effects on the Kagome Hubbard clusters. We use the numerical exact-diagonalization method with the Lanzos algorithm [15]. We employed the anti-periodic boundary condition to avoid excess degeneracy at the Γ point to reduce the finite-size effects (see Fig. 2). Our results for the magnetic field effect on the FBF of the 12-site (2x2 unit cells) cluster are shown in Table 1, where the total spins of the ground states are presented for the filling that equals or is slightly larger than half-filled where Mielke’s proof can be applied for the FBF at zero magnetic fields. We can see the ferromagnetic-paramagnetic transition induced by the magnetic field. The origin of the transition is the breakdown of the FB that produces the FBF. The FBF originates from a generalized Hund’s coupling, which results in a high-spin state. One may imagine that in a FB there exist localized states that are mutually disjointed. Remarkably, this does not hold for the FB of the Kagome lattice. Here the most compact states cannot be confined within the unit cell and must be overlapped with each other. The overlap between the compact states is advantageous for the high-spin states that exploit Pauli’s principle to avoid the repulsive interaction between electrons with opposite spins. However, if the FB is broken by the magnetic field, the single-particle energy of the high-spin states becomes larger than that of the low-spin state and the FBF is also broken by large magnetic fields. Here we note that the results for 3x2 unit cells are qualitatively the same as those for 2x2 unit cells.

Finally, we discuss the magnetoresistance when the FB crosses the Fermi level, calculating the Drude weight $D$, which is defined as the zero frequency part of the optical conductivity $\sigma(\omega) \equiv D\delta(\omega) + \text{regular part for finite } \omega$. The Drude weight is given by [15]

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

Here $\Psi_{0(n)}$ is the ground (n-th excited) state with 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, generally speaking, if $D = 0$, the system is insulating, while if $D > 0$ it is metallic (or superconducting). We present our results for the Drude weights of the ground states for Kagome clusters with 2x2 unit cells in the usual manner [13,14]: we also calculated the Drude weights for 3x2 unit cells and obtained qualitatively the same results as those for 2x2 unit cells. Figure 4 shows the magnetic field dependence of the Drude weight. Let us start from the case when the filling is away from half-filled on the FB. All data of the Drude weight are overlapped at $D = 0$, indicating the insulating behavior at zero magnetic field, and become finite, indicating the metallic behavior when the magnetic field is applied [Fig. 4(a)]. The metal-insulator transition induced by the magnetic field leads to the GNMR of the Kagome lattice. The GNMR is clearly understood within a single-particle picture. The group velocity of electrons is zero without the magnetic field and the system is insulating. In magnetic field the FB has a finite curvature and the group velocity becomes finite, resulting in a metallic system.

We also calculated the Drude weights at the half filled FB [Fig. 4(b)]. For small $U/t < 3.8$ [data for $U/t = 0.3$ in Fig. 4(b)] the magnetic field dependence is qualitatively the same as that for the case away from half filling. However, for large $U/t$ [data for $U/t = 5, 50, 100$ in Fig. 4(b)], we find the metal-insulator transition occurs simultaneously with the ferromagnetic-paramagnetic one for a magnetic field ($\phi = 1/8$). We can see for large $U/t$ that the high-spin ($S = 2$) and insulating states with negligible Drude weights below $\phi = 1/8$...
turn into the low-spin \((S = 0)\) and metallic states with finite Drude weights above \(\phi = 1/4\): at \(\phi = 1/8\) the data for \(U/t = 5, 50, 100\) are almost completely overlapped at \(D = 0\). Let us consider the physical picture for these simultaneous transitions. The electrons on the FB for the high-spin state have the same spin direction (defined as the up direction without any loss of generality). We should remember that the number of \(k\)-points and that of the electrons are exactly the same at half filling. Thus, all the up-spin states for the high-spin states are completely occupied at the half filling, while all the down-spin states are unoccupied. Thus, the up-spin electrons on the FB cannot move there because of Pauli’s exclusion principle and the absence of any spin-flipping processes in the present Hamiltonian. These are the reasons the high-spin states are insulating at half filling. Above \(\phi = 1/4\), the metallic states appear because there the ground states turn to low-spin ones where both unoccupied and occupied states co-exist for both up and down spins and electrons can now move, resulting in the simultaneous ferromagnetic-paramagnetic and metal-insulator transitions. On the other hand, we also note that the Drude weight is converged to a finite value for the large \(U/t\) limit for low-spin states: even above \(\phi = 1/4\), we indeed find the high-spin ground states for very large \(U/t\) (for e.g. \(U/t = 110\) at \(\phi = 1/4\)). Thus there may be no Mott transition for low-spin states in the usual sense even though the FB is half-filled. This is because the half-filling of the FB does not correspond to half-filling of the total system having multi-bands. This means that electrons can move, avoiding additional on-site interaction energy in real space. This situation is different from single-band Hubbard models at half filling. There 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 the first site to its nearest neighbor.

In conclusion, we have studied magnetic field effects on a 2D Kagome lattice. The Hofstadter butterfly shows wide gap structures that may be easily observable in real experiments through the wide plateaus of the QHE. On the flat band, the ferromagnetic-paramagnetic and metal-insulator transitions (GNMR) induced by the magnetic field are predicted. At the half-filled FB, we find the metal-insulator transition occurs simultaneously with the ferromagnetic-paramagnetic one for large \(U/t\) at a magnetic field. All of the above magnetic field effects should be observable for small (order of 0.1T) magnetic fields in quantum dot superlattices.

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[16] 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.
FIGURES

FIG. 1. The Kagome lattice structure and the magnetic flux though the Kagome lattice is schematically shown in Fig. (a). Figure (b) shows the single-particle energy levels in the magnetic field (i.e. Hofstadter butterfly).

FIG. 2. Single-particle band structure of the Kagome lattice without a magnetic field is shown.

FIG. 3. Hall conductance $\sigma_{xy}$ is shown for both $\phi = 1/8$ (a) and $\phi = 1/4$ (b) as a function of Fermi energy.

FIG. 4. Magnetic field dependences of the Drude weights of 12-site (2x2 unit cells) Kagome Hubbard cluster are shown. Figure (a) shows the results when the filling is away from half filling of the FB, while Fig. (b) shows those at half filling.
TABLES

TABLE I. Total spins of the ground state of the 12-site (2x2 unit cells) Kagome Hubbard cluster with $U/t = 5$ are shown as a function of the electron number $N$ and magnetic field $\phi$. 