Hofstadter butterfly in the Falicov–Kimball model on some finite 2D lattices

Subhasree Pradhan

Department of Physics, Indian Institute of Technology Kharagpur, Kharagpur 721302, India
Department of Physics, Jhargram Raj College, Jhargram, West Bengal 721507, India

E-mail: spradhan@phy.iitkgp.ernet.in

Received 8 June 2016, revised 9 September 2016
Accepted for publication 16 September 2016
Published 21 October 2016

Abstract
Spinless, interacting electrons on a finite size triangular lattice moving in an extremely strong perpendicular magnetic field are studied in comparison to a square lattice. Using a Falicov–Kimball model, the effects of Coulomb correlation, magnetic field and finite system size on their energy spectrum are observed. Exact diagonalization and Monte Carlo simulation methods (based on a modified Metropolis algorithm) have been employed to examine the recursive structure of the Hofstadter spectrum in the presence of several electronic correlation strengths for different system sizes. It is possible to introduce a gap in the density of states even in the absence of electron correlation, which is anticipated as a metal to insulator transition driven by an orbital magnetic field. With further inclusion of the interaction, the gap in the spectrum is modified and in some cases the correlation is found to suppress extra states manifested by the finite size effects. At a certain flux, the opened gap due to magnetic field is reduced by the Coulomb interaction. An orbital current is calculated for both the square and the triangular lattice with and without electron correlation. In the non-interacting limit, the bulk current shows several patterns, while the edge current shows oscillations with magnetic flux. The oscillations persist in the interacting limit for the square lattice, but not for the triangular lattice.

Keywords: Hofstadter butterfly, Falicov–Kimball model, electron correlation, orbital magnetic field

(Some figures may appear in colour only in the online journal)

1. Introduction

The problem of electrons moving in a periodic potential under the influence of a quantizing, perpendicular magnetic field has been rigorously investigated, giving rise to several phenomena such as the quantum Hall effect [1, 2], superconducting flux phases [3] and the famous Hofstadter butterfly [4], to name a few. This problem is characterized by two length scales, the periodicity of the lattice potential and the magnetic length. The regime where these two length scales are comparable to each other exhibits an interesting fractal like structure, the Hofstadter butterfly [4, 5]. The energy spectrum is found to depend critically on the ratio $pl/q$ ($p$ and $q$ are positive integers, the ratio of the magnetic flux per plaquette to the flux quantum). If $pl/q$ is a rational number, each energy band is split into $q$ subbands by the magnetic field, revealing a recursive structure. The movement of electrons in the external magnetic field is responsible for the broadening of the Hofstadter bands. The bands may eventually overlap and smear out the original fractal structure of the energy spectrum (see figure 1). There are a number of theoretical studies examining this fractal spectrum in the presence of several external parameters such as electron–phonon coupling [6, 7], disorder [8] and Rashba spin–orbit coupling [9]. Despite the simplicity of the problem, many aspects of it still remain unresolved due to the paucity of both experimental and exact theoretical results. The main challenge in realizing this recursive structure is the requirement of extremely high magnetic field. There are recent indications of this kind of structure in some artificial superlattices by enhancing the lattice scale to the magnetic length scale [10–12]. These systems, however, lack the adjustability of the lattice geometry and particle-particle interactions, which could
be overcome by a cold atom system in a defect-free environment. One of the major attainments in the cold atom experiment is the simulation of effective magnetic fields through laser assisted tunneling which go beyond the possibilities already offered by conventional condensed matter systems [13–15]. An optical lattice prepared by a periodic potential utilizing standing wave of light has been realized in lower as well as in higher dimensions experimentally. The fascinating nature of the butterfly is a characteristic feature of 2D systems. The self-similar fractal energy structure depends sensitively on the geometry of the underlying lattice, as well as the applied magnetic field. Triggered by the intriguing results on a square lattice, attempts to study tight-binding electrons in the presence of a perpendicular magnetic field on triangular lattice with hexagonal geometry [16–18] has revealed interesting physics. A triangular plaquette is a basic building block of geometrical frustration. Therefore, it would be interesting to see the effects of lattice geometry as well as the effects of the finite size of the systems on the energy spectrum. The latest advances in cold atom engineering in creating adjustable lattice geometries provide the opportunity to study the dependence of the Hofstadter butterfly on the lattice parameters. On the other hand, it is known that properties of low-dimensional systems may be highly affected by the presence of electronic correlations. Electronic correlation itself can induce several many-body effects like metal-insulator transitions, charge-density waves (CDW) and antiferromagnetism. Usually, the Hubbard model is chosen as the prototypical correlated system. However, one can also have two types of electrons, considered by Falicov and Kimball: a set of spinless fermions conventionally termed itinerant electrons, and a set of infinitely massive localized particles, described by the classical occupation variables \( n_f \); which take values 1 or 0 at a particular site. Each particle does not interact with particles of the same species, but there is an on-site interaction between itinerant and localized particles whose strength is given by the dimensionless constant \( U \). The Falicov–Kimball model (FKM) (and its extended version) is one of the simplest correlated models with nontrivial many-body correlation effects like metal insulator transition, CDW, superconductivity and ferroelectricity [19–23].

Moreover, recently there have been proposals for the realization of FKM in optical lattices with mixtures of light and heavy atoms [24, 25] in the context of cold atom systems. A gauge-field can be experimentally realized for ultracold particles (fermions and bosons) in optical lattices [26]. Several experiments in optical lattices have confirmed the Hofstadter physics [27]. The interaction between the light and heavy atoms is achieved experimentally either by a Feshbach resonance or by tuning the lattice potential height and thus allows one to study the correlation effects on the Hofstadter butterfly. Therefore, it is interesting to study the physics of correlated fermions in the context of the Hofstadter problem in an artificial triangular optical lattice. Electrons on a finite size square lattice in the presence of perpendicular magnetic field were studied in order to see the effects of boundary conditions and Hubbard type of Coulomb correlations recently [28]. There are interesting results on a Falicov–Kimball model in a square lattice in the presence of external magnetic field in the half-filled limit [29]. It is therefore interesting to study how the finite size and FKM–U would affect the energy spectrum, in particular the mid-gap energies. In order to incorporate finite size effects as well as on-site correlations on Hofstadter butterfly, an FKM on a finite system with both open and periodic boundary conditions is investigated on a non-bipartite lattice i.e. a triangular lattice and the obtained results are compared with the results for a square lattice. The remainder of the manuscript is organized as follows: in the next section the Hamiltonian is formulated in the presence of a magnetic field and results for a finite uncorrelated system with various boundary conditions are presented in the section 3. Section 4 verifies the flux phase theorem for spinless fermions in strong magnetic field in both the non-interacting as well as the interacting limit. The results showing the effects of electron correlation on the Hofstadter spectrum are discussed in section 5. Section 6 gives some results on current calculation on finite lattices. Conclusions follow in section 7.

2. Formulation

A spinless FKM is used to study the effect of Coulomb repulsion on the Hofstadter spectrum in different lattices. The Zeeman effect is ignored which effectively projects out the ‘wrong-spin’ sector to high energies at high magnetic fields.

\[
H_0 = -\sum_{\langle i,j \rangle} t_{ij} (d_i^\dagger d_j + h.c.) + U \sum_i d_i^\dagger d_i f_i^\dagger f_i + E_f \sum_i f_i^\dagger f_i,
\]

where, \( \langle i,j \rangle \) are the nearest-neighbour site indices on a square lattice (lattice constant \( a = 1 \)), \( d_i \) (\( f_i \)) are itinerant (localized) electron annihilation operators at the site \( i \). The first term is the kinetic energy due to hopping between nearest neighbours, where, \( t \) is the hopping integral for \( d \)-electrons (for the sake of simplicity, \( t = 1 \)). The second term represents on-site Coulomb interaction between \( d \) and \( f \)-electrons (at \( E_f \), with density \( \rho_f = \frac{1}{N} \sum_i f_i^\dagger f_i \), \( N \) being the number of sites). This Hamiltonian commutes with \( \hat{n}_{f,i} \), in which case local occupancy of \( f \)-electron is either 0 or 1. In the half-filled Falicov–Kimball model, the filling \( \rho \) is fixed as \( \rho = \rho_0 + \rho_f = 1 \).

When a uniform magnetic field normal to the plane of the lattice is switched on, the field couples to the spinless, mobile fermions via canonically conjugate momenta only. Zeeman coupling being absent, the field couples to the ‘orbital degrees’ and the orbital physics plays an important role in the present scenario. Because of the local gauge invariance, the external magnetic field couples to electrons through a well-defined ‘Peierls phase’ in the hopping matrix element of the Hamiltonian (equation (1)). With the choice of a Landau gauge \( \tilde{\mathbf{A}}(r) = (0, Bx) \), electrons propagating along \( x \) and \( y \) would acquire different phase shifts and a quantum interference occurs. While hopping in the \( y \)-direction, electron picks up a ‘Peierls phase’ \( t_y(\tilde{\mathbf{A}}) = -t \exp(\pm ie/h \int_0^{\tilde{\mathbf{A}}} A(r) dr) = -t \exp(\pm 2\pi im\tilde{\phi}/\phi_0) \).
\( \phi = B a^2 \) is the flux per plaquette of a square lattice which is the Aharonov–Bohm (AB) phase around a closed path through the plaquette. Lattice periodicity is lost along the \( x \)-direction due to the magnetic field. As is customary, the lattice is discretized by \((x, y) = (ma, nb)\)—each site is then indexed by integers \( (m, n) \) along \((x, y)\)-directions respectively. The Hamiltonian is invariant only for lattice translations in the magnetic translation group \([30]\). Only rational magnetic flux, i.e. \( \phi = \frac{p}{q} \phi_0 = \alpha \phi_0 \) with \( p, q \) are integers and relatively prime to each other, where the Dirac flux quantum is \( \phi_0 \), leads to a unit cell \( q \) times larger than the original one to accommodate an integer flux \( p \phi_0 \). Therefore, to enfold a magnetic flux \( B = \frac{2 e}{q} \), the magnetic supercell now becomes a strip of length \( L \) \([6]\) (in this calculation the maximum \( L = 48 \) is used). The energy spectra can be obtained efficiently by diagonalizing a \( L \times L \) matrix. In the non-interacting limit \((U = 0)\), the single particle spectrum displays a self-similar structure on a square lattice, the famous Hofstadter butterfly. As it is seen from figure 1, this fractal structure shows well-defined clear gaps, known as Hofstadter-gaps which appear and disappear depending on the rational values of the magnetic flux. Next, the same problem is formulated on a triangular lattice. The band dispersion without flux is given by \( E(k) = -2t(2 \cos \frac{k a}{2} \cos \frac{k b}{2} + \cos k a) \) and the atom at the origin has six neighbours at \((\pm a, 0)\), \((\pm a/2, \pm \sqrt{3} a/2)\) while \((k_a, k_b)\) represents the wave vector of an electron and \( a \) is the lattice constant. The band dispersion gives the allowed energies in the range \(-6t \leq E \leq 3t\) and the density of states has a logarithmic singularity at \( E = 2 \). With an asymmetric gauge, the corresponding tight-binding Hamiltonian reads as

\[
H = -t \sum_{m,n} (d^\dagger_{m+1,n} d_{m,n} \exp(i \alpha \phi)) + \text{h.c.} \\
- \frac{1}{2} \sum_{m,n} (d^\dagger_{m,n+1} d_{m,n} \exp(i \alpha \phi)) + \text{h.c.} \\
- \frac{1}{2} \sum_{m,n} (d^\dagger_{m,n,1} d_{m,n,1} \exp(i \alpha \phi)) + \text{h.c.}
\]

where,
\[
\alpha_{ij} = 0; \quad i = (m + 1, n), \quad j = (m, n) \\
\alpha_{ij} = 2 \pi m \varphi; \quad i = (m, n), \quad j = (m, n + 1) \\
\alpha_{ij} = (2 \pi m + 1/2) \varphi; \quad i = (m, n + 1), \quad j = (m + 1, n).
\]

The hopping parameter along the \( x \)-direction is \( t_1 \), along the \( \pm \pi/3 \) direction is \( t_2 \), and along the \( \pm 2 \pi/3 \)-direction is \( t_3 \). Due to a Peierls substitution in the tight-binding Hamiltonian for an electron in a triangular lattice, phases are associated with four nearest neighbour hoppings, which makes an angle \( \pm \pi/3 \) and \( \pm 2 \pi/3 \) with respect to the \( x \)-direction, respectively. The lattice is discretized by assuming \((x, y) = (mb, nc)\) where \( b = a/2 \) and \( c = \sqrt{3} a/2 \), \( \varphi = 2 \sqrt{3} B B^2 \phi_0 \) is the magnetic flux through each unit cell \([31]\). If the energy eigenvalues are plotted with respect to magnetic flux one observes the Hofstadter butterfly for the triangular lattice (see figure 2) \([16, 31]\).

![Figure 1.](image1.png) **Figure 1.** The Hofstadter butterfly: single particle energy spectrum as a function of magnetic flux per plaquette \( \alpha = p/q \) in an infinite square lattice.

![Figure 2.](image2.png) **Figure 2.** Tight binding dispersion of an infinite triangular lattice in a magnetic field with isotropic hopping \( t_1 = t_2 = t_3 = 1 \).

In the FKM, the interactions among two kinds of electrons, which are kinematically in nature, arises entirely from the Fermi statistics for a given \( f \)-electron configuration. The \( d \)-electrons sample the annealed disordered background of \( f \)-electrons \((n_{ij} = 0, 1 \) only\) and a Monte Carlo annealing over all possible \( f \)-electron configurations yields the ground state configuration. On the other hand, for a non-bipartite lattice considered here, particle-hole symmetry is no longer extant. The local conservation of \( f \)-electron number implies that the Hamiltonian \((1)\) can be written as

\[
H = - \sum_{ij \omega} \Delta \omega_d(d^\dagger_{i\omega} d_{j\omega}) + E_f \sum_i f^\dagger_i f_i ,
\]

where, \( \Delta \omega_d = - \sum_{ij \omega} t_{ij}(\vec{A}) + (U \omega_d - \mu) \sum d^\dagger_i d_i \).

Therefore, to obtain the spectrum of this Hamiltonian for different configurations \( \{ \omega \} \) of \( f \)-electrons by numerically diagonalizing the Hamiltonian over different \( \{ \omega \} \) and annealing over the
configurations. The partition function has the following form
\[ Z = \sum_{\omega} \text{Tr}(\exp(-\beta H(\omega))), \beta = \frac{1}{kT}. \]
In order to obtain the ground state, a simulated annealing is employed by ramping the temperature down from a high to a very low value. The process, therefore, involves the following steps: (i) the first step is to select a set of \( f \)-electron configurations \( \{\omega\} = \omega_1, \omega_2, \ldots, \omega_N \) for a fixed \( \rho_f \) (\( \rho_f = \rho - \rho_j \)). (ii) Fix the values of \( U, E_f \) and \( \alpha \), find the eigenvalues of \( H(\omega) \) and the corresponding total free energy \( F(\omega) = \frac{1}{\beta} \log Z \).

The chemical potential \( \mu \) is used to fix the \( d \)-electron number \( \rho_d \).

The corresponding total energy is then \( E(\omega) = \lim_{T \to 0} F(\omega) \). (iii) Generate a new random configuration \( \{\omega\} \) of \( f \)-electron and calculate the new energy \( E(\omega') \). (iv) Find \( \Delta E = E(\omega') - E(\omega) \) and compare \( s = \exp(-\beta \Delta E) \) with a random number \( r_\omega (0 < r_\omega < 1) \): if \( r_\omega < \min(1, s) \), accept the new configuration \( \{\omega\} \), else reject it. The steps (i) to (iv) are repeated until convergence is reached at a temperature \( T \). The temperature is then lowered down slowly to a very low value and at each step of \( T \), the same routine is performed. Repeating this few times usually leads to a unique low-energy state to the temperatures desired. Different kinds of moves have been employed to prevent the system to getting stuck to a local minima. The Monte Carlo simulation produces various charge ordered states of varying periodicities as a function of filling \( (\rho_j) \), \( U \) and \( \alpha \). A similar approach was employed in order to study the phase transitions in FKM on a square lattice earlier [32].

3. Finite size effects

With the choice of a Landau gauge, the \( y \)-directional hopping is associated with a phase which again depends on the \( x \)-component of the position vector ‘\( m' \). For a system with \( L \) sites, periodicity along \( x \) is retained at a magnetic field \( B = 2\pi L \). Due to the translational invariance in \( y \)-direction one can consider a plane wave along this direction. For a system with finite boundary, the plane wave vanishes at the system edges. With periodic boundaries on both the directions, the Hofstadter energy spectrum depends precisely on \( \alpha \). The Hofstadter spectrum with torus geometry i.e. a lattice with periodic boundary conditions (PBC) along both directions and rational magnetic flux through the plaquette, shows well-defined gaps. For rational \( \alpha \), the spectrum splits into \( q \) energy bands. When \( q \) is even, the two bands touch each other at \( E = 0 \) (see figure 1). Without PBC, although the qualitative aspect of the spectrum remains invariant for several kinds of boundaries, some extra states show up inside the Hofstadter gaps. The effects of lattice sizes on the energy spectrum for a triangular lattice is examined. As seen from figure 3 the spectrum contains some extra states (compare with figure 2) which survive even if the system size is increased from \( 9 \times 9 \) to \( 24 \times 24 \), although they become unimportant for systems with increasing size and vanish for an infinite system.
4. Flux phase theorem

Let us first consider the non-interacting limit. The flux phase conjecture [33, 34] states that the total energy of spinless non-interacting electrons at a uniform flux of $\frac{\alpha}{q}$ has an absolute minimum corresponding to a commensurate value of the flux per plaquette which is again related to the band-filling factor. In the $U = 0$ limit, the band filling is the same as $d$-electron density, found from the integrated density of states (DOS), using the formula:

$$\rho_\phi = \int_{\alpha}^\mu D(\varepsilon)\,d\varepsilon$$

(4)

here, $\varepsilon$ is the energy dispersion for a particular magnetic flux. The total energy for a fixed electron density is defined as

$$E_T(\alpha) = \int_{\alpha}^{\mu} \varepsilon D(\varepsilon)\,d\varepsilon.$$  

For a square lattice, the energy-minimizing flux per plaquette $\alpha = \frac{\pi}{q}$, exactly equals the electron density per site (see figure 4(i)) whereas for a triangular lattice, it occurs at a flux which is half of the electron-filling (see figure 4(ii)). For a square lattice, the absolute minimum in total energy occurs when the Fermi energy lies in a gap corresponding to a flux per plaquette $\alpha$ equal to the electron density per site i.e., $\rho_\phi$. Hence the energy is lowered by the lowest group of states just below the largest commensurability gap [34] at the lower energy side (see figure 1). For a half-filled ($\rho_\phi = 1/2$) triangular lattice, the total energy depicts an absolute minimum at $\alpha = 1/4$ (see figure 4(iii)), it is confirmed that the total energy $E_T(\alpha)$ of the 1/4 flux state is $-1.20$, which is substantially lower than the ground state energy $-0.98$ for the no-flux or $\pi$-flux state.

Later on, this conjecture was verified by Lieb [35] for a half-filled band along with the extension to several kinds of electron–electron interactions for a large class of Hamiltonians as well as to the higher dimensional geometries. The Lieb conjecture has been checked in this study for a half-filled bipartite as well as a non-bipartite lattice in the presence of FKM-type $d-f$ interaction; where the $d$-electron density is still fixed by equation (4). But the $f$-electron number being a classical variable, is fixed by the ratio of the total no of $f$-electrons to the total no of sites ($=N_f/N$). Even in the presence of interaction, at half-filling ($\rho = 1$), the energy is a minimum at half-flux for a square lattice, while for a triangular lattice it occurs at 1/4-flux; both identical to the corresponding non-interacting situation. Therefore, it is proved that this theorem is valid even in the presence of interaction (see inset (b) in figures 4(i) and (ii)). This rule checks out for all the cases discussed below.
5. Effects of electron correlation on the Hofstadter spectrum

For the half-filled (symmetric case: $\rho_0 = \rho_f = 0.5$) FKM, a square lattice has a charge-density-wave (CDW) ground state [36, 37]. The localized $f$-electrons fill up one of the two sublattices (the so called ‘chequerboard’ structure) and the corresponding ground state is insulating for any $U > 0$ and at sufficiently low $T$. For small $U$, one may treat the localized $f$-electron potential as a perturbation to the non-interacting band and then gaps do not open unless there is an electron density corresponding to a Fermi surface nesting as $\rho_f = 1/2$. A gap is an indication that the system is an insulator, for it implies that it costs more energy to put a particle into the system than is gained by removing one. The chequerboard is the only configuration for which precise nesting occurs. At half-filling, the spectrum is split down the middle: a gap opens up symmetrically about $E = 0$ in the Hofstadter spectrum (figure 5) for any $\alpha$ in a finite lattice and this gap has exactly the same value as $U$. The upper and lower halves of the spectrum are narrow, the sum of their widths less than the width for $U = 0$.

In the other case, a triangular lattice with geometric frustration leads to huge ground state degeneracies at low temperatures as the large $U$ expansion of FKM maps onto an Ising antiferromagnet in a magnetic field. Therefore, it is expected that the frustration has a bearing on the ground state $f$-electron configurations. From the Monte-Carlo simulation, as described in section 2, it is found that a half-filled triangular lattice shows different kinds of $f$-electron patterns for different values of $U$ and magnetic flux (figure 6). In the absence of an orbital field, the ground state of a half-filled FKM on triangular lattice has an irregular phase (figure 6(a)) for low $U$ regime: for some special flux values the Monte Carlo annealing results in some specific $f$-electron arrangements. The field promotes the ordered phases at $\alpha = 1/4, 1/3$ and 1/2, where axial and diagonal stripe patterns are formed. At high $U$-regime, the correlation wins over the magnetic field and the effective $f$-electron configuration is found to be a diagonal stripe (shown in figure 6(d)) which confirms earlier findings [38]. The ordered ground state configurations obtained at half-filling are used for the calculation. The structure of the Hofstadter butterfly is greatly modified while band-gaps and bandwidths are also modified under the effect of Coulomb repulsion (see figure 7, also compare with figure 2). With small $U$, the spectrum is distorted and a splitting occurs in the spectrum. This is visible clearly in figure 7, the region with no states increases with $U$. The spectrum has the symmetry $E(\alpha) = -E(1 - \alpha)$ seen in the figure as well. The diagonal region in the spectrum (lightly shaded region in figure 7), becomes narrower in the high-$U$ regime.

The normalized DOS (in figures 8 and 9) of $d$-electrons for various values of $U$ on a $48 \times 48$ lattice under both PBC and open boundary condition (OBC), show how several parts of the spectrum depend on the magnetic field, finite size and the magnitude of the Coulomb repulsion. When the flux changes, van Hove singularity peaks shift (compare figures 8(d) and (g)), and a pseudo gap or gap opens. The definition of gap parameter in FKM used here: $\Delta = E(N_0 + 1, N_f) + E(N_0 - 1, N_f) - 2E(N_0, N_f)$ (for a fixed $f$-electron number as a function of the magnetic field as well as $U$). For $B = 0$, electronic correlations open up a gap in the DOS (figures 8(c), 10(c) and (d)). On the other hand, even in the absence of electron correlation, one can see a gap induced in the DOS (at $\alpha = 0.5$) solely due to the external magnetic field (figure 8(j)). This is an example, where one can see the metal to insulator transition due to localization by an external magnetic field. There have been a number of earlier works suggesting magnetic field induced metal to insulator transition in diverse systems like quantum hall systems [39, 40], two dimensional electron system in silicon [41], quasi-1D and 2D systems threaded by flux [42] and in a loosely bound Holstein polaron [6]. There are theoretical reports of localization induced by random magnetic fields in a 2D non-interacting electronic system, confirmed by several groups [43]. In the context of 2D localization, magnetic fields can induce a metal-insulator transition by controlling the degeneracy of the Landau levels [44]. For weak to moderate Coulomb repulsion, the DOS strongly depends on the magnetic field. There are commensurability effects (as discussed in section 4); for a particular electron density the Fermi energy lies in a gap between subbands. For a triangular lattice with OBC, the magnetic field brings in extra states inside the Hofstadter-gaps, which have been shown in the DOS at some rational values of flux (it is evident for $\alpha = 1/2$ case, in figure 9).

The right columns in figures 8 and 9, show the gap induced by magnetic field (at $\alpha = 1/2$) is greatly modified by the Coulomb interaction $U$ (from top to bottom). After a certain $U$, the positions of the van Hove singularity show the appearance of two-satellite features on either side of the gap along with an increase of the band-width. This is driven by strong interaction and increasing $U$, the two bands merge and close the gap which opened due to the magnetic field (the gap is a true one for PBC, while there is small DOS for OBC). The same thing happens for a Falicov–Kimball model on a square lattice under orbital fields for $U \sim 4$ and 1/2-flux [28]. In a triangular lattice, as $U$ is increased, the lower edge of the lower band remains pinned, while the upper edge of the lower band and the entire upper band move and open up a gap in the DOS. Moreover, in the half-filled limit, the gap opens up at the Fermi level and drives the system to an insulator (with the Fermi level in the gap). The gap reduces (or closes) with $U$ (below $U \sim 4$), this is an example of insulating to a metallic transition by tuning the magnetic field (moving along the rows in figures 8 and 9). A somewhat similar situation exists for a magnetic-field induced transition from an Anderson insulator at $B = 0$ to a quantum Hall conductor in a disordered 2DEG system, explained by a model of magnetic-field-induced delocalization [45].

For a strong magnetic field the DOS becomes robust against Coulomb correlation. This result already suggests that the Coulomb interaction modifies various parts of the Hofstadter butterfly in different ways. As seen from the plot, states which appear due to the progressive vanishing of the finite size effects with the addition of Coulomb repulsion within the range of $U$ used (for some values of the flux). A further increase in $U$
Figure 6. Ground state configurations for localized $f$ electrons (black dots are the positions of the $f$-electrons) for $\rho_f = 1/2$, $U = 1$ and at (a) $\alpha = 0$, (b) $\alpha = 1/4$, (c) $\alpha = 1/3$ and (d) $\alpha = 1/2$.

Figure 7. Evolution of the Hofstadter spectrum in a finite triangular lattice (with OBC) as a function of $U$. (a) $U = 0$, (b) $U = 1.0$, (c) $U = 4.0$ and (d) $U = 8.0$. 

J. Phys.: Condens. Matter 28 (2016) 505502
causes an enhanced band gap. Although not shown here, at larger values of $U$ no further qualitative change in the DOS occurs, except a larger band gap and narrower bandwidth. The gap in figure 10 corroborates what is already observed in figures 8 and 9: $\Delta$ varies differently in the presence or absence of on-site correlation. In the $U = 0$-limit, $\Delta/t$ has a maximum at $\alpha = 0.5$ (figure 10(a)), this trend is retained for $U = 1$, although the gap reduces in almost all cases, except for some
special values of flux. The opposite happens (figure 10(b)) at the same place for large \( U \); at \( \alpha = 1/2 \), the gap has the lowest value. In the absence of magnetic field, \( \Delta \) increases with \( U \) exponentially. However, in the presence of the field there is a gap even when \( U = 0 \) (figure 10(d)). This gap is induced by the field, again this gap reduces at some \( U \), although at high \( U \), the variation of gap with \( U \) more or less follows the same pattern as in figure 10(c).

### 6. Orbital current

Recent experiments have explored effects of artificial orbital magnetic fields [27, 46, 47] on cold atoms (bosons and fermions). Such gauge fields can result in equilibrium charge currents of electrons. These currents can be measured by a ‘unidirectional quench’ method, which provides a decrease in the particle hopping amplitude in one direction across the entire lattice. This is achieved simply by tuning the optical lattice laser intensity along a certain direction. By tracking the subsequent space-time variation of the density for this quench protocol, for both bosons and fermions, one can probe bulk as well as edge current patterns which convert current patterns into experimentally measurable real-space density pattern [48]. The expectation value of such a current is an useful quantity for rotating quantum systems [49].

There is a protocol of site-resolved measurement of current statistics for ultrascold bosons subject to gauge field in one as well as two-dimensions in optical superlattices [50]. It is interesting to study the different current patterns for fermions in a strong orbital field in a finite size system and hence to see the effects of FKM-type correlation on these currents.

The introduction of the magnetic field in the hopping term of the Hamiltonian of equation (1) breaks the temporal invariance, thus causing an imbalance between currents entering and leaving different sites. At zero magnetic field the system has time translational invariance and the net current of the charged particles is zero because of the equally probable reversed paths. Even for a small value of magnetic flux the time invariance is suddenly broken and the reversal paths are no more equally probable; in fact only one of the two reversal paths is permitted; the other one corresponds to change of the sign of the magnetic flux \( \alpha \).

From the continuity equation, the local bond current operator is defined as,

\[
\nu_{ij} = \frac{1}{i\hbar} \left[ t_{ij} d^\dagger d_j - t^\dagger_{ij} d^\dagger d_i \right];
\]

a bond connecting neighbouring sites \((i,j) = (n,m; n,m \pm 1)\) of the lattice.

The corresponding current statistics for an \( 8 \times 8 \) square lattice are summarized in figure 11. Note that for a square lattice, calculations are performed in the interval \( \alpha = (0 – 0.5) \), as the Hamiltonian is invariant under \( \alpha \rightarrow 1 – \alpha \), while \( \alpha \rightarrow -\alpha \) only changes the magnetic field direction. Figure 11 shows the current profile in the ground state for different interaction strengths and \( U \) values for a square lattice. In figures 11(a) and (b), current flows in anti-clockwise direction, in (c) and (e) the central current reverses sign and in (f) the central as well as the bulk current change sign. The current patterns found for all \( U \) (not shown) look similar to those obtained at \( U = 0 \). The bulk current reverses sign beyond some critical flux \( \alpha \sim 0.43 \), and this value is same for all \( U \). The same calculation is done on a triangular lattice for which \( E(\alpha) = -E(1-\alpha) \) with \( 0 \leq \alpha \leq 1/2 \), with an additional bond taken along the diagonal. Figure 12 shows current configurations for some commensurate flux in a \( 12 \times 12 \) triangular lattice in the non-interacting as well as finite-\( U \) regime at half-filling. As seen in figure 12(a), with increased \( U \), the current avoids the sites which are occupied by \( f \)-electrons and flows though a narrow channel (figures 12(c) and (d)).

Another useful observable, the edge current for a finite size system, is defined as,

\[
\Lambda_C \equiv \sum_{(i,j) \in C} \nu_{ij},
\]

counted in an anticlockwise direction along boundary \( C \). The total current along the boundary \( \Lambda_C \), for a square lattice (in figure 13) shows an oscillation with \( \alpha \) and becomes maximum at \( \alpha = 0.25 \). In the presence of \( U \): a reduction in the magnitude of edge current is observed, but the pattern of oscillation is fixed in all cases. The edge current contributed from the extra states in a finite size lattice, is reduced with a Coulomb correlation which is already demonstrated in a previous section: a repression of extra states as a result of high-\( U \). As there is a change of sign of current at about \( \alpha \sim 0.43 \), the same is reflected for the boundary current; at this flux, the edge current goes to zero and reverses sign. For this flux, there is a change in the rotational symmetry of a (nondegenerate) ground state, which occurs due to a level crossing or avoided level crossing corresponding to eigenstates of rotational symmetry. Since the effect exists even when \( U = 0 \) and in the bulk too, it is connected to the change in symmetry of
the wave function. There are similar results on currents in a Bose Hubbard model on a finite square lattice [50] as well as in rotating square lattices [49]. The current rotates in the opposite direction at some specific range of flux. This happens due to change in symmetry of the wave function at that point (e.g. $2\pi j$ is the allowed rotations for a square, with $j = 1 \cdots 4$). Beyond this $\alpha$, the edge current almost becomes negligible and goes to zero at $\alpha = 0.5$, indicating that there is metal to insulator transition induced by magnetic field in a square lattice. Edge current in figure 14 in a triangular lattice at half-filling shows that the variations in current becomes smoother with interactions and changes sign around $\alpha = \frac{2}{3}$. The change in ground state rotational symmetry and the associated level crossing leads to the current changing sign for the triangular lattice too.

7. Summary and conclusion

The finite size effects on a Hofstadter butterfly for a triangular lattice in the presence of Coulomb interaction is investigated and compared with the earlier results for a square lattice.
There is an interplay between the applied magnetic field and the electronic correlation. The magnetic field induces a gap (largest at $\alpha = 0.5$) in the density of states even in the absence of correlation, such an observation highlights the metal to insulator transition due to localization by orbital magnetic field. At finite $U$, however, this gap is suppressed from its $U = 0$ value and becomes almost zero at $\alpha = 0.5$ for an infinite system and the gap reappears for larger $U$. For a finite size system, the Hofstadter gaps are filled up with some extra states and these states go away with the inclusion of correlation in some cases.

Acknowledgments

The author acknowledges useful discussions with A Taraphder, Monodeep Chakraborty, M M Maska, Diptiman Sen, S Lal and R Ganesh. The Centre for Theoretical Studies, IIT Kharagpur, is acknowledged for providing computer facilities.
References

[1] Thouless D J, Kohmoto M, Nightingale M P and Nijs M D 1982 Phys. Rev. Lett. **49** 405
[2] Rammal R, Toulouse G, Jaekel M T and Halperin B I 1983 Phys. Rev. B **27** 5142
[3] Lederer P, Poilblanc D and Rice T M 1989 Phys. Rev. Lett. **63** 1519
[4] Hofstadter D R 1976 Phys. Rev. B **14** 2239
[5] Langbein D 1969 Phys. Rev. **180** 633
[6] Pradhan S, Chakraborty M and Taraphder A 2016 Phys. Rev. B **93** 115109
[7] Berciu M 2010 Phys. Rev. B **82** 201102R
[8] Zhou C, Berciu M and Bhatt R N 2005 Phys. Rev. B **71** 125310
[9] Hofstadter D R 1976 Phys. Rev. B **14** 2239
[10] Melinte S et al 2004 Phys. Rev. Lett. **92** 036802
[11] Dean C R et al 2013 Nature **497** 598
[12] Albrecht C, Smet J H, Klitzing K V, Weiss D, Umansky V and Schweizer H 2001 Phys. Rev. Lett. **86** 147
[13] Folling S, Gerbier F, Widera A, Mandel O, Gericke T and Bloch I 2005 Nature **434** 481
[14] Greiner M, Mandel O, Esslinger T, Hansch T W and Bloch I 2002 Nature **39** 315
[15] Bloch I, Dalibard J and Zwerger W 2008 Rev. Mod. Phys. 80 885
[16] Claro F H and Wannier G H 1979 Phys. Rev. B **19** 6068
[17] Hatsugai Y and Kohmoto M 1990 Phys. Rev. B **42** 8282
[18] Gumbs G and Fekete P 1997 Phys. Rev. B **56** 3787
[19] Falicov L M and Kimball J C 1959 Phys. Rev. Lett. **22** 997
[20] Freericks J K and Zlatić V 2003 Rev. Mod. Phys. **75** 1333
[21] Freericks J K and Falicov L M 1990 Phys. Rev. B **41** 2163
[22] Remirez R and Falicov L M 1971 Phys Rev. B **3** 2425
[23] Pradhan S and Taraphder A 2016 J. Phys.: Conf. Ser. at press
[24] Ates C and Ziegler K 2005 Phys. Rev. A **71** 063610
[25] Ziegler K 2007 J. Nucl. Phys. A **790** 718c
[26] Dalibard J, Gerbier F, Giedminas J and Patrik O 2011 Rev. Mod. Phys. **83** 1523
[27] Aidselsburger M, Atala M, Lohse M, Barreiro J T, Paredes B and Bloch I 2013 Phys. Rev. Lett. **111** 185301
[28] Czajka K, Gorka M and Mierzejewski M 2006 Phys. Rev. B **74** 125116
[29] Wrobel M, Mierzejewski M and Maska M M 2010 Acta Phys. Pol. A **118** 79
[30] Zaks I 1964 Phys. Rev. **136** 776
[31] Oh G Y 2000 J. Korean Phys. Soc. **37** 534
[32] Maska M and Czajka K 2006 Phys. Rev. B **74** 035109
[33] Affleck I and Marston J B 1988 Phys. Rev. B **37** 3774
[34] Hasegawa Y, Lederer P, Rice T M and Wiegmann P B 1989 Phys. Rev. Lett. **63** 907
[35] Lieb E H 1994 Phys. Rev. Lett. **73** 2158
[36] Brandt U and Schmidt R Z 1990 Phys. B **79** 295
[37] Brandt U and Melsch C Z 1989 Phys. B **75** 365
[38] Yadav U K, Maitra T, Singh I and Taraphder A 2011 Europhys. Lett. **93** 47013
[39] Laughlin R B 1981 Phys. Rev. B **23** 5632
[40] Halperin B I, Lee P A and Read N 1993 Phys. Rev. B **47** 7312
[41] Popovie D, Fowler A B and Washburn S 1997 Phys. Rev. Lett. **79** 1543
[42] An J, Gong C D and Lin H Q 2001 Phys. Rev. B **63** 17443
[43] Furusaki A 1999 Phys. Rev. Lett. **82** 604
[44] Abrahams E et al 2001 Rev. Mod. Phys. **73** 251
[45] Jiang H W, Johnson C E, Wang K L and Hannahs S T 1993 Phys. Rev. Lett. **71** 1439
[46] Lin Y J, Compton R L, Jimenez-Garcia K, Porto J V and Spielman I B 2009 Nature **462** 628
[47] Rom T, Best Th, Oosten D V, Schneider U, Folling S, Paredes B and Bloch I 2006 Nature **444** 733
[48] Killi M and Parmeckantini A 2012 Phys. Rev. A **85** 061606
[49] Bhat R, Holland M J and Carr L D 2006 Phys. Rev. Lett. **96** 060405
[50] Kellner S and Marquardt F 2014 Phys. Rev. A **89** 061601