

Electronic structure of the Falicov-Kimball model with a magnetic field: Dynamical mean-field study

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The two-dimensional Falicov-Kimball model in the presence of a perpendicular magnetic field is investigated by the dynamical mean-field theory. Within the model the interplay between electron correlations and the fine electron structure due to the magnetic field is essentially emerged. Without electron correlations the magnetic field induces the electron structure to the so-called Hofstadter butterfly. It is found that when electron correlations drives the metal-insulator transition, they simultaneously smear out the fine structure of the Hofstadter butterfly. In a long-range ordered phase, the electron correlation induced gap preserves the fine structure, but it separates the Hofstadter butterfly into two wings.

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I. INTRODUCTION

The problem of electrons moving under an external magnetic field has attracted a lot of attention since the beginning of quantum mechanics. Two-dimensional electron gas under a perpendicular magnetic field creates the quantum Hall effect.¹⁻⁴ It comprehensively deals with the interplay of electron correlations and magnetic field. The integer quantum Hall effect is due to the quantization of the energy levels of free electrons under a magnetic field,^{1,2} while the fractional quantum Hall effect is essentially due to the electron interaction under a magnetic field.^{3,4} The picture totally becomes complex when electrons move additionally on a lattice or under a periodic potential. The simultaneous presence of magnetic field and lattice potential gives the spectra of two-dimensional noninteracting electrons a fine structure of the famous Hofstadter butterfly.⁵ The Hofstadter butterfly displays a recursive structure over rational gauge field and a Cantor set at any irrational gauge field. The Hall conductance of the noninteracting Bloch electrons is still quantized with an integer number when the Fermi energy lies within a gap of the Hofstadter butterfly.⁶ When electron correlations are included, the effect of simultaneous presence of magnetic field and electron interaction on the lattice band energy is not fully understood yet. Without the external field electron correlations can induce different phenomena, for instance, the metal-insulator transition, long-range ordered phases. When electron correlations are absent, the magnetic field creates the Hofstadter butterfly of the electron structure. A simultaneous presence of electron correlations and magnetic field would induce a complexity of the electron structure. The exact diagonalization of finite lattices shows that the electron correlations smear out the Hofstadter butterfly.⁷ However, it is not easy to distinguish the fine electron structure due to the presence of magnetic field from the discrete energy levels due to the finite-size effect of the exact diagonalization. The Hartree-Fock mean-field calculations reveal the electron structure with the Hofstadter butterfly and an additional correlation induced gap.^{8,9} It gives rise to an interest in the study of the interplay between electron correlations and magnetic field in a two-dimensional lattice beyond the Hartree-Fock approximation and in the thermodynamic limit. In experi-

mental aspect, with the rapid development of ultracold technique some fundamental models of many quantum particles can be realized by loading ultracold particles into optical lattices (see, for example, the review in Ref. 10). In particular, by using the technique of laser-assisted tunneling¹¹ or of lattice rotating¹² artificial gauge fields can be created in optical lattices. As a result it is possible to realize the effect of magnetic field on the Bloch electrons by loading ultracold particles into optical lattices with artificial gauge field. Indeed, recently several models of optical lattices were proposed to study the Hofstadter butterfly of ultracold particles.^{11,13-15}

In the present paper, we theoretically study the effect of electron correlations on the Hofstadter butterfly of the electron structure under a magnetic field. The electron correlations are modeled by the Coulomb interaction of the Falicov-Kimball model (FKM).¹⁶ It is a local repulsive interaction of mobile electrons and massive localized particles. The FKM was originally introduced to describe a metal-insulator transition in transition-metal oxides. It can be viewed as a simplified Hubbard model where electrons with down spin are frozen and do not hop. The FKM was also used as a starting point to investigate different electron correlation phenomena, for instance the mixed valence¹⁷ or the electronic ferroelectricity.^{18,19} The FKM can also be incorporated into different models to study various aspects of electron correlations such as the charge-ordered phase in manganese compounds²⁰⁻²² or electron localization.^{23,24} Much progress has been made on solving the FKM in both exact and approximation ways, where all properties of the conduction electrons are well known.²⁵⁻²⁸ In the homogeneous phase the FKM displays a metal-insulator transition. When the Coulomb interaction is strong, it prevents the mobility of itinerant electrons by forming the Mott-Hubbard gap. At low temperature a charge ordering occurs. For half filling the charge ordering gap opens at the Fermi level and drives the system into an insulating phase. One may expect that the electron correlation induced gaps of the Mott-Hubbard type and of long-range charge ordering may have different effects on the fine structure of the Hofstadter butterfly. A realization of the FKM was also proposed as an optical lattice of a mixture of light fermionic atoms (e.g., ⁶Li) and heavy fermionic atoms

(e.g., ^{40}K).^{29,30} When the optical lattice modeling the FKM is established, it is also possible to create an artificial magnetic field. In the present paper, the two-dimensional square lattice with a perpendicular magnetic field is considered. The dynamical mean-field theory (DMFT) is employed to calculate the electron structure of the considered model. The DMFT is widely and successfully applied to study strongly correlated electron systems.^{31,32} It gives the exact solutions in infinite dimensions. However, for two-dimensional systems the DMFT is just an approximation. It neglects nonlocal correlations. However, the applications of the DMFT to FKM show that the approximation is still accurate in two dimensions.^{33,34} We find that the electron correlation effect on the Hofstadter butterfly depends on the nature of the correlated phase when the magnetic field is absent. When any long-range order is absent, electron correlations only induce the metal-insulator transition and they smear out the fine structure of the Hofstadter butterfly. In a long-range ordered phase, the electron correlation induced gap preserves the fine structure, but separates the Hofstadter butterfly into two wings.

The plan of the present paper is as follows. In Sec. II we describe the FKM with a perpendicular magnetic field on a square lattice. We also present the DMFT for calculating the Green function in this section. In Sec. III the numerical results are presented. Finally, the conclusion and remarks are presented in Sec. IV.

II. FALICOV-KIMBALL MODEL WITH A PERPENDICULAR MAGNETIC FIELD AND THE DYNAMICAL MEAN-FIELD THEORY

In this section, we present the DMFT for the Falicov-Kimball model in the presence of a magnetic field. The model is described by the following Hamiltonian

$$H = - \sum_{\langle i,j \rangle} t_{ij} c_i^\dagger c_j - \mu \sum_i c_i^\dagger c_i + E_f \sum_i f_i^\dagger f_i + U \sum_i c_i^\dagger c_i f_i^\dagger f_i, \quad (1)$$

where $c_i^\dagger (c_i)$, $f_i^\dagger (f_i)$ are the creation (annihilation) operators for itinerant and localized electrons at site i , respectively. t_{ij} is the hopping integral of itinerant electrons between site i and j . U is the local interaction of itinerant and localized electrons. μ is the chemical potential for itinerant electrons and E_f is the energy level of localized electrons. We will consider only the half filling case, where $\mu = -E_f = U/2$. In the presence of a magnetic field the hopping integral acquires the Peierls phase factor³⁵

$$t_{ij} = t \exp \left(i \frac{2\pi}{\phi_0} \int_{\mathbf{R}_i}^{\mathbf{R}_j} \mathbf{A} \cdot d\mathbf{l} \right), \quad (2)$$

where $\phi_0 = hc/e$, and \mathbf{A} is the vector potential. For a constant magnetic field perpendicular to the square lattice, the Landau gauge can be chosen for the vector potential $\mathbf{A} = (0, Bx, 0)$, where B is the magnetic field strength. With this Landau gauge the hopping integral in the x direction is just t , while in the y direction it acquires additional phase factor $t \exp(\pm i 2\pi \alpha x_i)$, where $\alpha = Ba^2/\phi_0$, a is the lattice constant,

and x_i is the lattice site position in the x axis. In the following, we will set $a=1$. Parameter α is just the magnetic flux per unit cell in the units of the flux quantum ϕ_0 . It is clear that the Hamiltonian is invariant with the translation $\alpha \rightarrow \alpha + m$, where m is an integer. Therefore, it is only necessary to consider $0 \leq \alpha \leq 1$.

We will also only consider the rational magnetic field, i.e., $\alpha = p/q$, where p, q are two coprime integers. The translation operator that moves q lattice spacing in the x direction leaves the Hamiltonian unchanged. We divide the lattice into q penetrating sublattice in x direction, i.e., each lattice site can be indexed by a number n , and its coordinates x, y , where $n = \text{mod}(R_x, q)$, ($1 \leq n \leq q$). We take the Fourier transformation from the direct lattice to the reciprocal lattice

$$c_{n\mathbf{k}} = \frac{1}{\sqrt{N/q}} \sum_{xy} c_{nxy} e^{ik_x x + ik_y y},$$

where N is the number of lattice sites. The wave vectors k_x, k_y are restricted to the reduced Brillouin zone

$$-\frac{\pi}{q} \leq k_x \leq \frac{\pi}{q}, \quad -\pi \leq k_y \leq \pi.$$

The hopping part of Hamiltonian in Eq. (1) can be rewritten as

$$H_t = \sum_{\mathbf{k}} \hat{X}_{\mathbf{k}}^\dagger \hat{E}(\mathbf{k}) \hat{X}_{\mathbf{k}}, \quad (3)$$

where $\hat{X}_{\mathbf{k}}^\dagger = (c_{1\mathbf{k}}^\dagger, \dots, c_{q\mathbf{k}}^\dagger)$, and

$$\hat{E}(\mathbf{k}) = -t \begin{pmatrix} \varepsilon_{1k_y} & e^{-ik_x} & 0 & 0 & \dots & 0 & e^{ik_x} \\ e^{ik_x} & \varepsilon_{2k_y} & e^{-ik_x} & 0 & \dots & 0 & 0 \\ 0 & e^{ik_x} & \varepsilon_{3k_y} & e^{-ik_x} & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \dots & \vdots & \vdots \\ e^{-ik_x} & 0 & \dots & \dots & \dots & e^{ik_x} & \varepsilon_{qk_y} \end{pmatrix}, \quad (4)$$

with $\varepsilon_{nk_y} = \cos(k_y + (n-1)2\pi/q)$.

We apply the DMFT to the calculation of the Green function of itinerant electrons in the matrix form

$$\hat{G}(\mathbf{k}, \omega) = \langle \langle \hat{X}_{\mathbf{k}} | \hat{X}_{\mathbf{k}}^\dagger \rangle \rangle_\omega = [\omega + \mu - \hat{E}(\mathbf{k}) - \hat{\Sigma}(\omega)]^{-1}, \quad (5)$$

where $\hat{\Sigma}(\omega)$ is the self energy. Within the DMFT the self energy is independent on momentum. Moreover, it is also diagonal, i.e., $\Sigma_{nm}(\omega) = \delta_{nm} \Sigma_n(\omega)$. This formulation is similar to the DMFT applications for the antiferromagnetic or checkerboard charge-ordered phases.³² Basically, the DMFT is exact in infinite dimensions. However, its application for two-dimensional systems is just approximation. The approximation neglects nonlocal correlations which exist through the momentum dependence and off-diagonal elements of the self energy. The DMFT calculations for two-dimensional FKM without the magnetic field show that the approximation still accurate for the electron dynamics.^{33,34}

The self energy $\Sigma_n(\omega)$ is self consistently determined from the dynamics of a single interaction site embedded in an effective mean-field medium. For the FKM the effective

single-site problem can be solved exactly.²⁸ We obtain the Green function of the single-site problem²⁸

$$G_n(\omega) = \frac{W_{n0}}{\mathcal{G}_n^{-1}(\omega)} + \frac{W_{n1}}{\mathcal{G}_n^{-1}(\omega) - U}, \quad (6)$$

where $\mathcal{G}_n(\omega)$ is the Weiss field for sublattice n . The weight factors W_{n0} and W_{n1} can be calculated from the Weiss field

$$W_{n1} = f(\tilde{E}_n), \quad (7)$$

$$W_{n0} = 1 - W_{n1}, \quad (8)$$

where $f(\omega) = 1/[\exp(\omega/T) + 1]$ is the Fermi-Dirac distribution function, and

$$\tilde{E}_n = E_f - \int \frac{d\omega}{\pi} f(\omega) \text{Im} \log \left(\frac{1}{1 - U\mathcal{G}_n(\omega)} \right). \quad (9)$$

The Weiss field $\mathcal{G}_n(\omega)$ also satisfies the Dyson equation of the effective single-site problem, i.e.,

$$G_n^{-1}(\omega) = \mathcal{G}_n^{-1}(\omega) - \Sigma_n(\omega). \quad (10)$$

The single-site Green function for each sublattice in Eq. (6) can be interpreted as a superposition of two contributions of the lower and upper bands, separated by U . The self-consistent condition requires that the Green function obtained from the effective single-site problem must coincide with the local Green function, i.e.,

$$G_n(\omega) = \frac{1}{N/q} \sum_{\mathbf{k}} G_{nn}(\mathbf{k}, \omega). \quad (11)$$

With this self-consistent condition the system of equations for the self energy is closed. We can solve the system of equations by iterations as usual.²⁸

III. NUMERICAL RESULTS

In this section, we present the numerical results obtained by solving the DMFT equations by iterations. We take $t=1$ as the energy unit. The magnetic field parameter $\alpha=p/q$ varies with $p=0, 1, \dots, q$. We take $q=40$ in the numerical calculations. When p and q are not coprime, we can reduce them to coprime integers. This also reduces the matrix dimension of the Green function and saves the computation time. First, we consider the high-temperature phase, where the metal-insulator transition of the Mott-Hubbard type occurs. We emphasize that in this phase temperature does not affect on the electron structure. The phase is just the homogeneous solution of the DMFT equations and it is stable at high temperature. The electron structure can be imaged by using the density plotting of the density of states (DOS) of the itinerant electrons. In Fig. 1 we plot the image of the DOS for various values of U . It shows that the electron structure mimics the Hofstadter butterfly when electron correlations are included. For weak interactions the fine structure of the Hofstadter butterfly still survives. However, the electron correlations already smear out it. Some fine gaps in the structure of the Hofstadter butterfly are closed. As the value of U increases,

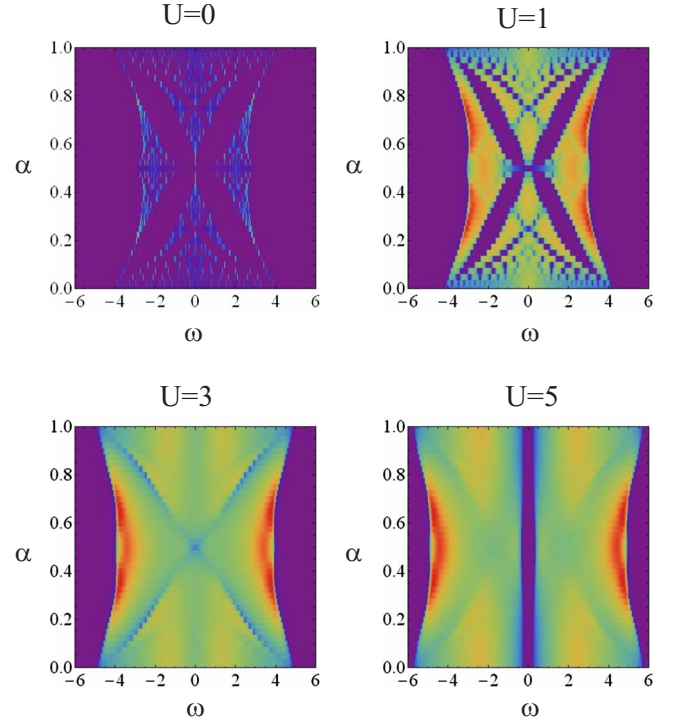


FIG. 1. (Color online) The density plot of the DOS of itinerant electrons of the high-temperature phase ($T=1$) for various values of U . The magnetic field parameter $\alpha=p/q$ varies with $p=0, 1, \dots, q$, and $q=40$. The color scheme corresponds to the rainbow color scheme, i.e., the red (violet) color corresponds to the largest (smallest) value of the DOS. In the black and white print, the black (dark-gray) color corresponds to the smallest (largest) value of the DOS.

the smearing becomes stronger. For strong interactions all fine gaps are closed. However, a middle rough gap opens for $U > U_c \approx 4t$. This gap is essentially the Mott-Hubbard gap, which opens in the insulating phase. Without the magnetic field the metal-insulator transition occurs at U_c . In the presence of the magnetic field the metal-insulator transition still occurs, but the lower and upper bands mimic the Hofstadter butterfly. The electron structure is symmetry in respect to lines $\omega=0$ and $\alpha=1/2$ like the noninteraction case, i.e., $\rho(\omega, \alpha) = \rho(-\omega, \alpha) = \rho(\omega, 1-\alpha)$, where $\rho(\omega, \alpha) = -\Sigma_n \text{Im} G_n(\omega)/q\pi$ is the DOS of itinerant electrons.

In Fig. 2 we plot the DOS of itinerant electrons for various values of α and U . When the electron correlations are absent ($U=0$) the number of bands is just q .⁵ One can observe that the q bands can be grouped into subgroups of bands which are separated by moderate gaps. Within a band subgroup the bands are also separated by fine gaps. For example, when $\alpha=3/8$, there are three subgroups of bands, one at $\omega=0$, and two others around $\omega = \pm 2$. When the interaction is included, the band number is reduced by closing the gaps. As the interaction increases, first the fine gaps within the band subgroups are closed, and then the gaps between the band subgroups are closed. In the insulating phase all the gaps in the Hofstadter butterfly are closed, but the Mott-Hubbard gap opens. The metal-insulator transition occurs at the same value of U for all values of the magnetic field. Despite of closing of the fine gaps in the insulating phase,

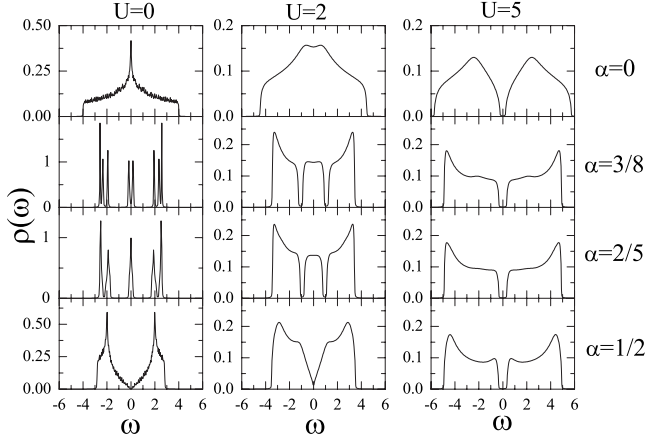


FIG. 2. The DOS of itinerant electrons of the high-temperature phase ($T=1$) for various values of α and U .

the intensity of the DOS of itinerant electrons still shows a mimic Hofstadter butterfly with smearing out fine features, as shown in Fig. 1. The smearing of the fine structure of the Hofstadter butterfly can be interpreted as a result of disorder average over all possible configurations of the localized particles in the homogeneous phase. Each magnetic band equally gets contributions from lower and upper Hubbard bands [see Eq. (6), and in the homogeneous phase $W_{n0} = W_{n1} = 1/2$]. As a consequence of the superposition of the two Hubbard band contributions, the magnetic bands are broadened. This also smears out the fine structure of the Hofstadter butterfly.

Without magnetic field the FKM also displays the checkerboard charge ordering at low temperature for any interaction $U \neq 0$. We study the possibility of the charge ordering when the magnetic field is present. In this case, we additionally divide the lattice into two penetrating sublattices in the y direction. If q is an odd integer, we double the value of p and q that $\alpha = 2p/2q$ and the checkerboard charge ordering is commensurate with the magnetic structure. In Fig. 3 we plot the image of the total DOS of itinerant electrons in the

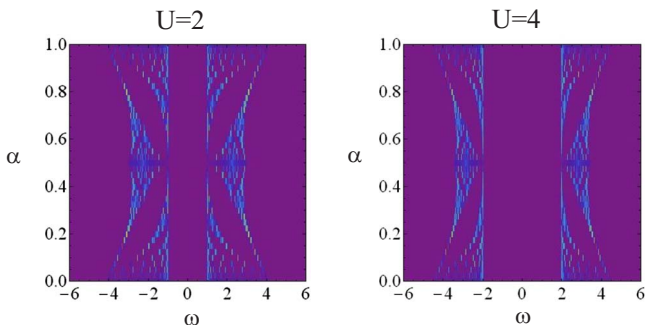


FIG. 3. (Color online) The density plot of the DOS of itinerant electrons of the charge-ordered phase at low temperature ($T=0.01$) for various values of U . The magnetic-field parameter $\alpha = p/q$ varies with $p=0, 1, \dots, q$, and $q=40$. The color scheme corresponds to the rainbow color scheme, i.e., the red (violet) color corresponds to the largest (smallest) value of the DOS. In the black and white print, the black (dark-gray) color corresponds to the smallest (largest) value of the DOS.

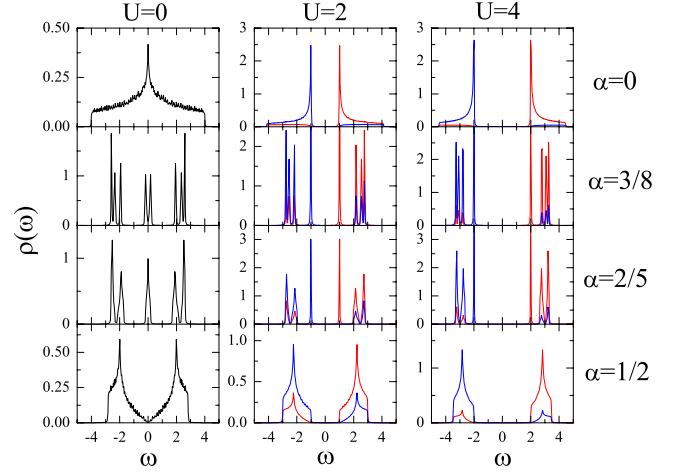


FIG. 4. (Color online) The DOS of itinerant electrons of the checkerboard charge-ordered phase at low temperature ($T=0.01$) for various values of α and U . The red (gray) and green (black) color lines corresponds to the DOS of two penetrating sublattices of the checkerboard charge-ordered phase.

checkerboard charge-ordered phase. It shows that the fine structure of the Hofstadter butterfly still remains, however, it is separated by a middle gap. The middle gap is the charge ordering gap, which locks itinerant electrons into the checkerboard charge pattern. As the interaction increases the charge ordering gap also increases and the band width of the lower and upper bands are slightly reduced. The preservation of the fine structure of the Hofstadter butterfly was also observed within the Hartree-Fock mean-field calculations.^{8,9} Within the mean-field analysis the recursion relation of the energy bands due to the magnetic field can be decoupled from the long-range order contributions.⁸ As a result, the fine structure of the Hofstadter butterfly is preserved. However, the Hartree-Fock mean-field approximation cannot find the smearing of the Hofstadter butterfly due to electron correlations in the absence of any long-range ordered phase. One can see from Eq. (6) in the charge-ordered phase each magnetic band gets only one contribution of the lower or upper Hubbard bands ($W_{n1} = 1$ or $W_{n1} = 0$). There is no a superposition of the lower and upper Hubbard band contributions. As a consequence, the magnetic bands cannot be smeared, unlike in the homogeneous phase.

In Fig. 4 we also plot the DOS of itinerant electrons of the two penetrating sublattices of the checkerboard charge-ordered phase for various values of U and α . It shows that the magnetic field does not affect on the charge ordering gap. The gap solely depends on the interaction as in the case of absence of the magnetic field. When q is even, the number of bands is also q , such as the noninteraction case. However, unlike the noninteraction case, the subgroup of bands at the Fermi level is separated by the charge ordering gap. When q is odd, the band at the Fermi level is split into two bands which are also separated by the charge ordering gap, as shown in Fig. 4 (the case $\alpha=2/5$ for example). The gaps between subgroups of bands are slightly reduced as the interaction increases.

We have only considered the symmetric half filling case. It is well known that away from half filling and in the ab-

sence of magnetic field the localized particles form at low temperature the complex charge patterns.^{25–27} The charge patterns may be periodic or separated depending on the model parameters. In the presence of the magnetic field the periodic charge patterns may preserve the fine structure of the Hofstadter butterfly, because there is no a superposition of the lower and upper Hubbard contributions in the local Green function, like in the checkerboard charge-ordered phase. However, the Hofstadter butterfly may be separated into different parts. In the separated phase the electron structure may become complicated. It requires a further study.

IV. CONCLUSION

In the present paper, we study the effect of electron correlations on the Hofstadter butterfly which is the electron structure of the two-dimensional Bloch electrons under a perpendicular magnetic field. By employing the DMFT we calculate the Green function of itinerant electrons in the case of rational magnetic field. Electron correlations exhibit different effects on the Hofstadter butterfly depending on the nature of the correlated phase when the magnetic field is absent. In the absence of any long-range order, electron correlations also induce the metal-insulator transition when the magnetic field is present. However, the electron correlations smear out the

fine structure of the Hofstadter butterfly. The number of bands is reduced as the interaction increases. In the insulating phase, all fine gaps of the Hofstadter butterfly are closed, but the Mott-Hubbard gap opens at the Fermi level. In a long-range ordered phase, the electron correlation induced gap, such as the checkerboard charge ordering gap in the FKM, preserves the fine structure of the Hofstadter butterfly. However, the Hofstadter butterfly is separated into two wings by the long-range ordering gap.

In the present paper, we have only considered the rational magnetic field. In the noninteraction case an irrational magnetic field induces the Hofstadter butterfly in the form of a Cantor set. The magnetic structure is incommensurate with the lattice structure as well as with the checkerboard charge ordering pattern. The effect of electron correlations on such Hofstadter butterfly remains open and we leave it for further study.

Recently, we became aware of the article of Wrobel *et al.*³⁶ in which the same model was studied and similar results were obtained by Monte Carlo simulations on finite lattices.

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