Hofstadter butterfly for a finite correlated system

Katarzyna Czajka, Anna Gorczyca, Maciej M. Maśka, and Marcin Mierzejewski

Department of Theoretical Physics, Institute of Physics, University of Silesia, 40-007 Katowice, Poland (Received 5 May 2006; revised manuscript received 21 June 2006; published 27 September 2006)

We investigate a finite two-dimensional system in the presence of an external magnetic field. We discuss how the energy spectrum depends on the system size, boundary conditions, and Coulomb repulsion. On one hand, using these results, we present the field dependence of the transport properties of a nanosystem. In particular, we demonstrate that these properties depend on whether the system consists of an even or an odd number of sites. On the other hand, on the basis of exact results obtained for a finite system, we investigate whether the Hofstadter butterfly is robust against strong electronic correlations. We show that for sufficiently strong Coulomb repulsion, the Hubbard gap decreases when the magnetic field increases.

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I. INTRODUCTION

The problem of electrons moving in a periodic potential under the influence of an external magnetic field has been investigated since the beginning of quantum mechanics. Despite the seeming simplicity of the problem, many of its aspects still remain unresolved. Even in the absence of electronic correlations, solutions are known only in limiting cases. In particular, two-dimensional (2D) electron gas under the influence of a periodic potential and a perpendicular magnetic field can be described in two limits: one of a weak periodic potential and the other of a strong periodic potential. In the former case, the applied magnetic field is the main factor that determines the behavior of electrons. As a result, the electronic wave functions are Landau-level-type, with the degeneracy lifted by the periodic potential. If the potential is modulated in one dimension, the width of the resulting "Landau bands" oscillates with the magnetic field as a consequence of commensurability between the cyclotron diameter and the period of potential modulation. It leads to oscillations in magnetoresistance, known as the Weiss oscillations.¹ If the potential is modulated in two dimensions, "minigaps" open in the "Landau bands," and the energy spectrum plotted versus the applied field is composed of the famous Hofstadter butterfly.^{2,3} It is interesting that the same spectrum occurs in a complementary limit, when the lattice potential is very strong, and the electronic wave functions are Blochtype, modified by the magnetic field.²

The simplest model for the case, when an applied field and a lattice potential are present simultaneously, is commonly referred to as the Hofstadter or Azbel-Hofstadter model.^{3,4} The corresponding Hamiltonian describes electrons on a two-dimensional square lattice with nearest-neighbor hopping in a perpendicular uniform magnetic field. The Schrödinger equation takes the form of a one-dimensional difference equation, known as the Harper equation (or the almost-Mathieu equation).^{3,5,6} It is also a model for a onedimensional electronic system in two incommensurate periodic potentials. The Harper equation also has links to many other areas of interest, e.g., the quantum Hall effect,⁷ quasicrystals, localization-delocalization phenomena,^{8,9} the noncommutative geometry,¹⁰ the renormalization group,^{11,12} the theory of fractals, the number theory, and the functional analysis.¹³ It is also useful in determining the upper critical field^{14–17} and the pseudogap closing field ¹⁸ in high-temperature superconductors.

The unusual structure of the Hofstadter butterfly is a characteristic feature of 2D systems. Similarly to the case of Landau levels, the dimensionality of the system is of crucial importance for the Hofstadter butterfly. The movement of electrons along the external magnetic field would be responsible for the broadening of the Hofstadter bands. They eventually may overlap and, in this way, smear out the original fractal structure of the energy spectrum. On the other hand, it is known that electronic properties of low-dimensional systems may be completely changed by the presence of electronic correlations. In particular, it is well known for 1D systems that perturbation theory breaks down and arbitrarily weak on-site Coulomb repulsion qualitatively changes the whole excitation spectrum from the Fermi- to Luttingerliquid type. The role of Coulomb interaction in the case of 2D lattice has intensively been investigated in connection with high-temperature superconductors. Although a complete description of the correlated 2D system is still missing, it became obvious that mean-field approaches are invalid even for moderate values of Coulomb repulsion. Therefore a question arises as to whether the fine structure of the Hofstadter butterfly is robust against the presence of electronic correlations. This problem has previously been investigated on a mean-field level.^{19,20} In particular, the analysis presented in Ref. 20 suggests that also in the presence of electronic correlations, the energy levels should form the Hofstadter butterfly with additional energy gap in the middle of the energy spectrum. However, the above-mentioned limitations of the mean-field results clearly show that these results do not represent a conclusive solution. In this paper we address this problem with the help of a method that is particularly suited for investigations of the low dimensional correlated systems, i.e., exact diagonalization of finite clusters. Although in this method short-range electronic correlations are exactly taken into account, finite-size effects will seriously affect the energy spectrum. These modifications can be of special importance when the system is under the influence of a magnetic field.^{21,22} In order to separate the correlations and sizeinduced effects, we start our investigations with a finite uncorrelated system and discuss both fixed (fbc) and periodic boundary conditions (pbc). Apart from the discussion of the

Hofstadter butterfly, these results may be applicable to investigations of nanosystems in the presence of a magnetic field, where fixed boundary conditions are more appropriate than the periodic ones.

II. FINITE-SIZE EFFECTS

For the sake of completeness, we start with a brief derivation of the Harper equation for the gauge $\mathbf{A}=B[-ay,(1-a)x,0]$. Here, the parameter $a \in (0,1)$ allows one to distinguish between the Landau (a=0) and symmetric (a=1/2) gauges. The 2D square lattice in the presence of an external, perpendicular magnetic field can be described by the tight-binding Hamiltonian

$$H = t \sum_{x,y,\sigma} \left(e^{i\phi_{x}y} c^{\dagger}_{(x,y)\sigma} c_{(x-1,y)\sigma} + e^{-i\phi_{x}y} c^{\dagger}_{(x,y)\sigma} c_{(x+1,y)\sigma} \right. \\ \left. + e^{-i\phi_{y}x} c^{\dagger}_{(x,y)\sigma} c_{(x,y-1)\sigma} + e^{i\phi_{y}x} c^{\dagger}_{(x,y)\sigma} c_{(x,y+1)\sigma} \right), \tag{1}$$

where $c^{\dagger}_{(x,y)\sigma}$ creates an electron with spin σ at the site (x,y)and *t* is the nearest-neighbor hopping integral in the absence of a magnetic field. $\phi_x = 2\pi\alpha a$, $\phi_y = 2\pi\alpha(1-a)$, and $\alpha = \Phi/\Phi_0$, where Φ is the magnetic flux through the lattice cell and Φ_0 is the flux quantum. In order to determine the eigenfunctions of this Hamiltonian, formally one should solve a 2D eigenproblem. However, in the case of the Landau gauge (*a*=0), the hopping integrals in Eq. (1) depend solely on the *x* coordinate. Because of the translational invariance along the *y* axis, eigenfunctions exhibit a planewave behavior in this direction $[\exp(iky)]$. This argumentation can be extended to a more general gauge. Such an extension requires an appropriate shift of the momentum *k*. For an $N_x \times N_y$ lattice with pbc, we introduce fermionic operators $c^{\dagger}_{x,k,\sigma}$ defined by

$$c^{\dagger}_{(x,y)\sigma} = \frac{1}{\sqrt{N_y}} \sum_{k} e^{-iy(k+\phi_x x)} c^{\dagger}_{x,k,\sigma}.$$
 (2)

The Hamiltonian (1) can then be written,

$$H = t \sum_{x,k,\sigma} \left[c_{x,k,\sigma}^{\dagger} c_{x+1,k,\sigma} + c_{x,k,\sigma}^{\dagger} c_{x-1,k,\sigma} + 2\cos(k - 2\pi\alpha x) c_{x,k,\sigma}^{\dagger} c_{x,k,\sigma} \right].$$
(3)

The resulting Hamiltonian is diagonal in the quantum numbers k and tridiagonal in the x coordinates. It means that the applied 1D transformation to the momentum space allows one to reduce the original 2D eigenproblem [Eq. (1)] to a 1D one. In the following, we study whether such a reduction is possible also for a finite system with fixed boundary conditions. The relevant wave function in this case is no longer the plane wave since it must vanish at the system edges. It is easy to check that the Hamiltonian of a 1D chain with fbc can be diagonalized with the help of the transformation $c_{y,\sigma}^{\dagger} \sim \Sigma_k \sin(ky) c_{k,\sigma}^{\dagger}$. In the case of a 2D lattice in the presence of the external magnetic field, an appropriate shift of the wave vectors allows one to cancel the Peierls phase factors for the hopping along the y axis,

$$c^{\dagger}_{(x,y)\sigma} = \sqrt{\frac{2}{N_y + 1}} \sum_{k} \sin(ky) c^{\dagger}_{x,k,\sigma} e^{2\pi i \alpha x y},$$

where the wave vectors

$$k = \frac{\pi}{N_y + 1}, \frac{2\pi}{N_y + 1}, \dots, \frac{N_y \pi}{N_y + 1}.$$

In the above equation we have assumed a=1. The generalization to the arbitrary value of a is straightforward.

The orthogonality relation

$$\sum_{y} \sin(ky) \sin(py) = \frac{N_y + 1}{2} \delta_{kp}.$$

allows one to carry out the inverse transformation. Then, the Hamiltonian takes the form

$$H = t \sum_{k,\sigma} \left[\sum_{x=1}^{N_x - 1} \sum_{y=1}^{N_y} \frac{2}{N_y + 1} \sum_p \sin(ky) \sin(py) \right]$$
$$\times (e^{-2\pi i \alpha y} c^{\dagger}_{x,k,\sigma} c_{x+1,p,\sigma} + \text{H.c.})$$
$$+ \sum_{x=1}^{N_x} 2 \cos(k) c^{\dagger}_{x,k,\sigma} c_{x,k,\sigma} \right].$$

Only the term responsible for the hopping along the y axis is diagonal in k, whereas the remaining hopping term is generally not. Therefore, contrary to the case of infinite lattice with pbc, the Hamiltonian cannot be reduced to a form that is diagonal in wave vectors and tridiagonal in real-space coordinates. The only exceptions occur for $\alpha=0$ and $\alpha=1/2$. The first case is trivial. In the latter case ($\alpha=1/2$), an additional transformation

$$c_{x,k,\sigma} \to \frac{1}{2} c_{x,k,\sigma} [1 + (-1)^x] - \frac{1}{2} c_{x,\pi-k,\sigma} [1 - (-1)^x],$$

leads to the Hamiltonian in the form given by Eq. (3). However, since $k \in (-\pi, \pi)$ for pbc and $k \in (0, \pi)$ for fbc, also in this case the energy spectrum depends on the boundary conditions. Consequently, degeneracy of the energy levels is lower for fbc than for pbc. An additional difference, which immediately follows from the analytical calculations, is related to the density of states $\rho(\epsilon)$ for $\alpha = 1/2$. In the case of an infinite system with pbc $\rho(0)=0$, whereas for a finite lattice with fbc, there exists an eigenvalue $\epsilon = 0$, provided the system consists of an odd number of sites. The proof of this statement is straightforward and, therefore, we omit the details. The difference between systems with an even and odd number of sites will be discussed in more detail in connection with the transport properties. In Fig. 1 we compare the density of states obtained for various boundary conditions and lattice sizes. It has been calculated using the standard formula

$$\rho(E) = -\frac{1}{\pi N_x N_y} \sum_n \Im \frac{1}{E - \varepsilon_n + i\eta},\tag{4}$$

where ε_n is the energy of the *n*th one-particle eigenstate.

In the presence of a magnetic field, the translation group of the lattice does not represent a symmetry group of the Hamiltonian and one can discuss periodicity only with re-



FIG. 1. (Color online) Density of states $\rho(E)$ as a function of the magnetic field (α) calculated with fixed (left column) and periodic (right column) boundary conditions [see Eq. (4)]. The brighter colors correspond to the larger values of the density of states. The first, second, and third rows show the results obtained for a 6×6 , 12×12 , and 30×30 cluster, respectively. The broadening of the one-particle levels η =0.05*t* has been assumed. In the last row, we magnify the regions marked above. In order to demonstrate the presence of the edge states, the broadening has been reduced to η =0.005*t*.

spect to the magnetic translation group.^{23,24} Consequently, for a finite system one can apply the pbc only for some particular values of α , which are determined by the system size. On the other hand, for fbc the energy levels can be calculated for an arbitrary magnetic field, as was demonstrated in Ref. 22. However, in order to directly compare the results obtained for fbc and pbc, in both cases we have used

only these values of the magnetic field, which are allowed for pbc. In the case of fbc there exist edge states, which are responsible for additional levels inside the energy gaps in the Hofstadter butterfly.²⁵ They are clearly visible in Fig. 1 in the density of states obtained for a 6×6 system. The relative contribution of these states to $\rho(\epsilon)$ decreases with the system size. Therefore, they are much less visible in the density of



FIG. 2. (Color online) Field dependence of the transport current through the 5×5 and 6×6 nanosystems coupled to macroscopic leads for the applied voltage eV=0.01t. $I_0=2et/h$, where *e* is the elementary charge and *h* is the Planck constant. See Fig. 5 in Ref. 26 for parameters and the details of the coupling between the nanosystem and the electrodes. The inset shows the field dependence of the one-particle eigenenergies located in the vicinity of E=0 obtained for an isolated nanosystem with fbc.

states obtained for larger systems and become unimportant for an infinite lattice. However, for a finite system, they may qualitatively change the well-known structure of the Hofstadter butterfly obtained from the Harper equation.

Transport properties

The above discussion can directly be applied to the investigations of transport properties of nanosystems. The fieldinduced modifications of the energy spectra lead to strong changes of the transport current, at least in the low-voltage regime. We use the formalism of nonequilibrium Green functions to analyze these effects in a nanosystem coupled to leads. The coupling is described by

$$H_{\text{nano-el}} = \sum_{\mathbf{k}, x, y, \alpha, \sigma} (g_{\mathbf{k}, x, y, \alpha} d^{\dagger}_{\mathbf{k}, \sigma, \alpha} c_{(x, y)\sigma} + \text{H.c.}), \qquad (5)$$

where $d_{\mathbf{k},\sigma,\alpha}^{\dagger}$ creates an electron with momentum **k** and spin σ in the electrode α . Here, $\alpha \in \{L, R\}$ indicates the left or right electrode. We assume a simple model in which the leads are described by a 2D lattice gas and the hopping between the leads and nanosystem is possible only perpendicularly to the edge of the nanosystem. $g_{\mathbf{k},x,y,\alpha}$ is nonzero only for sites (x, y), which are located at the edge α of the nanosystem. The details of calculations can be found in Refs. 26 and 27. Figures 2 and 3 show the field dependence of the transport current for various sizes of the nanosystem.

Two main features arise from the presented results: (i) strong magnetoresistance in a weak field regime and (ii) even-odd parity effect. Both these features occur for a low voltage only. The first effect is shown in Fig. 2. It can easily be understood on the basis of the field dependence of the one-particle energies that are close to the Fermi energy, as presented in the inset in Fig. 2. One can see that for low voltage, the number of states that participate in the transport



FIG. 3. (Color online) The upper panel shows the field dependence of the transport current through the 5×5 and 6×6 nanosystems for the applied voltage eV=0.01*t*. The lower panel shows the results obtained for 9×9 and 10×10 nanosystems with eV=0.002*t*. The remaining parameters are the same as in Fig. 2.

decreases when the magnetic field increases. This effect is due to a field-induced splitting of a strongly degenerated level at zero energy. This degeneracy, in turn, is a remanent of the van Hove singularity, that is, a typical feature of an infinite 2D lattice. There is, however, a significant difference between systems with an even and odd number of lattice sites. In the former case, a strong magnetic field can completely remove states from the vicinity of the Fermi energy, which results in the vanishing of the current. On the other hand, if there is an odd number of lattice sites, one state is always located at zero energy. As a result, a finite conductivity occurs for an arbitrary magnetic field. This parity effect originates from the facts that the energy spectrum is symmetric with respect to the zero energy and the number of energy levels is equal to the number of lattice sites. The difference between systems consisting of an even and odd number of sites is pronounced for $\alpha = 1/2$, which can be seen in Fig. 3. The even-odd parity effect is a well-known feature of persistent currents in mesoscopic rings, where it occurs due to its nontrivial first homotopy group.²⁸ Here, we have demonstrated that a similar effect may also occur in a nanosystem with a trivial topology: in an isolated nanosystem as well as in a system coupled to macroscopic leads. In the first case it shows up in the energy spectrum, whereas in the latter case it



FIG. 4. Density of states obtained for a 2×3 cluster with fbc for various values of the Coulomb repulsion and the magnetic field.

is visible also in the transport properties. An additional similarity between rings and the systems under investigation concerns the fact that the parity effect occurs only in small systems and disappears in the thermodynamic limit.

III. ROLE OF CORRELATIONS

After establishing the role of boundary conditions and its significance for the properties of nanosystems, we switch to the main question, whether the Hofstadter energy spectrum is robust against the presence of strong electronic correlations. Both the external magnetic field and electronic correlations give rise to the opening of the energy gaps in the density of states. One could expect that these mechanisms should independently contribute to the opening of these gaps. In the following, we demonstrate that this intuitive statement is wrong and, actually, the external magnetic field reduces the Hubbard energy gap. In order to investigate this problem, we consider the 2D Hubbard model in the presence of the magnetic field

$$H_{\text{Hubb}} = H_{\text{kin}} + U \sum_{x,y} n_{(x,y)\uparrow} n_{(x,y)\downarrow}, \qquad (6)$$

where the kinetic term is given by Eq. (1) and the electronnumber operator $n_{(x,y)\sigma} = c^{\dagger}_{(x,y)\sigma}c_{(x,y)\sigma}$. In the following, we investigate the half-filled case, when the Hubbard gap opens at the Fermi level, driving the system from a metallic state to an insulating one.

This Hamiltonian has been diagonalized most often by means of the Lanczös method. It is one of the most effective computational tools for searching for the ground state and some low-lying excited states of a finite system. We start with a system sufficiently small to allow one to determine the whole energy spectrum. In the case of finite system calculations pbc can be applied only for specific values of the magnetic field, which depend on the cluster size. Therefore, in the following we use the fbc. Figure 4 shows how the density of states depends on the magnetic field and the magnitude of the Coulomb repulsion. One can see that for weak to moderate Coulomb repulsion, its influence on the density of states strongly depends on the applied magnetic field. In the absence of a magnetic field (α =0), even relatively weak electronic correlations (U=2t) strongly modify the energy spectrum. On the other hand, for a strong magnetic field the density of states becomes robust against the Coulomb correlations. In particular, for $\alpha = 1/2$, densities of states obtained for U=0 and U=2t hardly differ from each other. This result already suggests that the Coulomb interaction modifies various parts of the Hofstadter butterfly in a different way. It remains in contradiction to the results obtained in the meanfield analysis.²⁰ In the latter approach the Coulomb repulsion opens an almost-field-independent gap in the middle of the Hofstadter butterfly. Additionally, the one-particle energies remain in the range (-4t, 4t), at least for moderate U, i.e., the electronic correlations do not change the spectrum width. It has also been reported in Ref. 20 that for stronger Coulomb repulsion the only modifications of the Hofstadter butterfly concern the larger band gaps and narrower bandwidths. Contrary to the mean-field results, the exact diagonalization method indicates that electronic correlations lead to a substantial modification of the density of states. First, there is excitation beyond the range (-4t, 4t). When U increases, the one-particle excitations are replaced by the collective ones with a finite live time. Instead of the δ -like peaks in the density of states, we obtained a much larger number of wider peaks, which eventually may overlap. Therefore, we expect that electronic correlations smear out the fine structure of the Hofstadter butterfly.



FIG. 5. (Color online) Magnitude of the reduced Hubbard gap $[\Delta^*(U, \alpha)]$ as a function of U for various magnetic fields. These results have been obtained for a 12-site cluster with fbc.

For application purposes, the most important property concerns the density of states in the vicinity of the Fermi level. Therefore, we restrict the following study only to the ground state and the lowest excited states. We analyze the field dependence of the Hubbard gap $\Delta(U, \alpha)$ that opens in the middle of the density of states. In Fig. 5. we present a reduced gap $\Delta^*(U, \alpha) = \Delta(U, \alpha) - \Delta(U, 0)$, whereas $\Delta(U, 0)$ is presented in the inset of this figure.

As one could expect, Δ increases with U for an arbitrary magnetic field. However, the negative slope of Δ^* as a function of U clearly indicates that this increase is smaller when the magnetic field is switched on. Finally, for sufficiently strong Coulomb repulsion, the Hubbard gap seems to be a monotonically decreasing function of the magnetic field for $\alpha \in (0, 1/2)$. Since the Hamiltonian is invariant under the transformation $\alpha \rightarrow 1-\alpha$, the gap monotonically increases with α , for $\alpha \in (1/2, 1)$. This monotonic behavior is an unexpected result that strongly contrasts with the uncorrelated case, where the gap changes irregularly (discontinuously) with magnetic field, as can be inferred from Fig. 1.

The Hubbard model has already been applied for investigations of nanosystems, e.g., molecular wires²⁷ and quantum dot arrays (see Ref. 29 for a detailed discussion and estimation of the relevant model parameters). The latter case is of particular interest since the size of the elementary cell can be adjusted in such a way that the flux through the cell can be of the order of the flux quantum and then, the structure of the Hofstadter butterfly may be visible. Unfortunately, the present approach is probably oversimplified for a quantitative description of electronic correlation in the quantum-dot arrays, where one should account for a large number of states per dot. In spite of this, the considered Hubbard Hamiltonian allows for at most two electrons per site. Additionally, we have restricted our considerations to only the on-site repulsion U, which corresponds to the intradot interaction. In a more realistic approach, an extended multiband Hubbard model with intersite interaction should be used, but such extensions are presently beyond the reach of the exact diagonalization techniques.

IV. SUMMARY

The structure of the Hofstadter butterfly arises due to the coexistence of the periodic potential and the perpendicular magnetic field in the 2D electron gas. It is well known that the presence of Coulomb interaction in low-dimensional systems is responsible for the strong modification of its electronic properties. Motivated by these facts, we have investigated how the butterfly structure is affected by the correlations. In contrast to the mean-field results, we have demonstrated that Coulomb correlations are responsible for broadening of the quasiparticle levels. As a result, some of the Hofstadter bands overlap, and the fractal butterfly structure smears out. We have shown that for sufficiently strong repulsion the Hubbard gap monotonically decreases with the external magnetic field for $\alpha \in (0, 1/2)$. This result strongly contrasts with the irregular behavior of the density of states in the uncorrelated case. Unfortunately, beyond the meanfield level, results can be obtained only for relatively small systems. We expect, however, that similar changes occur also in much larger systems. On the other hand, some of the results can directly be applied to the investigations of the nanosystem, e.g., quantum-dot arrays. The finite-size effects seriously modify field dependence of its transport properties. Similarly to the persistent currents in nanoscopic and mesoscopic rings, transport currents are also different in systems consisting of an odd and even number of sites.

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