Hofstadter butterfly for the hexagonal lattice

Godfrey Gumbs* and Paula Fekete
Department of Physics and Astronomy, Hunter College of the City University of New York, 695 Park Avenue, New York, New York 10021
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A theoretical investigation is presented for the energy spectrum of two-dimensional Bloch electrons subject to a periodic modulation in both lateral directions for a lateral surface superlattice with hexagonal symmetry. The calculation is carried out for a single band in the tight-binding approximation in the presence of a perpendicular magnetic field. The Peierls' substitution is applied and the resulting Schrödinger equation is solved when the magnetic flux through a unit cell is a rational fraction ($\alpha = p/q$) of the flux quantum ($\phi_0 = h/e$). The energy spectrum is obtained numerically and results are presented for several values of the in-plane wave vector **k** and the overlap integral between nearest-neighbor lattice sites.
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I. INTRODUCTION

The problem for the electronic properties of a two-dimensional (2D) electron system (ES) under the influence of both a periodic potential and a perpendicular magnetic field has long been a fascinating subject in theoretical solid state physics. The solution to this problem has been approached in two fundamentally different ways. One is the semiclassical, or low-field method, based on the Peierls-Onsager assumption.[1,2] This method is applicable in the limit of weak magnetic fields and introduces a single-band effective Hamiltonian for Bloch electrons in a perpendicular magnetic field. The second method is a quantum mechanical approach introduced by Rauh, Wannier, and Obermair[3] and is suitable for strong magnetic fields and uses the free-electron Landau eigenstates as a basis and the periodic lattice potential as a perturbation.

So far, there has been a considerable amount of work which has been carried out to explore the energy spectrum of Bloch electrons in either a weak magnetic field or Landau quantized electrons in a weak 2D lattice potential. Since the publication of the first papers in this field by Azbel[4] (strong magnetic field limit with a weak lattice potential treated as a perturbation) and Hofstadter[5] (strong lattice potential with a weak magnetic field), there has been continuously growing interest in this field. In addition to the theoretical work on the subject, recent advances in submicrometer lithography and nanofabrication techniques have made it possible to create lateral surface superlattices with modulation periods much shorter than the elastic mean free path but comparable with the cyclotron radius at low magnetic fields, thereby making it possible for experimentalists to find indications of the Hofstadter spectrum[6–8] and its effect on the transport and optical properties of 2D ES.[9,10]

The early theoretical[5] and experimental[11,12] work focused on square lattices. However, it was not evident whether the conclusions for the square lattice would be valid for the hexagonal and triangular lattices. The energy spectrum for the tight-binding Hamiltonian for a hexagonal lattice was investigated by Langbein[13] and Claro and Wannier.[14] Sometime later, Hasewaga, Hatsugai, Kohmoto, and Montambaux[15] calculated the 2D electronic energies in a perpendicular magnetic field for the square, triangular, and honeycomb lattices for various values of the overlap integrals for the wave functions. Recently, Kuhn *et al.*[16,17] calculated the Landau level spectrum of a 2D ES in a lateral surface superlattice with hexagonal symmetry using the Landau eigenfunctions as a basis set and diagonalizing the coefficient matrix for a predetermined subset of the basis. The problem of the energy spectrum for electrons on a hexagonal lattice in the tight-binding approximation in a perpendicular magnetic field is far less explored than the square lattice. The purpose of this paper is to complement this study for this case, thereby extending the work of Claro and Wannier[14] for the hexagonal lattice to include the effect of anisotropic hopping on the lattice and to examine the effect on the energy spectrum for a finite lattice wave number. To put the problem in perspective, we briefly review the relevant literature.

There have been three limiting situations in the study of 2D ES in a periodic potential and a perpendicular magnetic field. When the strength of the potential is large compared to the cyclotron energy, one follows Hofstadter[5] by using a single-band Hamiltonian obtained by the Peierls' substitution. This approach was further developed by Schellnhuber and Obermair[18] who included a perturbation term given by the Fourier expansion of the lattice potential which yielded the tight-binding Hamiltonian as the lowest-order approximation. Claro[19] used this approach to examine the effects due to the next-nearest neighbors on the energy spectrum of a square lattice in a perpendicular magnetic field. Another approach has been presented by Thouless[20] who compared the energy spectra of the anisotropic triangular and square lattice with nearest-neighbor coupling with the isotropic square lattice with next-nearest-neighbor coupling. Further contributions to the improvement of the tight-binding formalism have been made by Zak[21] who used group theory to explain the splitting of the energy bands into magnetic subbands within the framework of an effective Hamiltonian formalism.

On the other hand, when the potential strength is much less than the cyclotron energy, the problem can be solved by using free electron Landau eigenstates as a basis set for diagonalizing the Hamiltonian. This is the approach followed by Rauh[22] in calculating an upper bound for the width of the

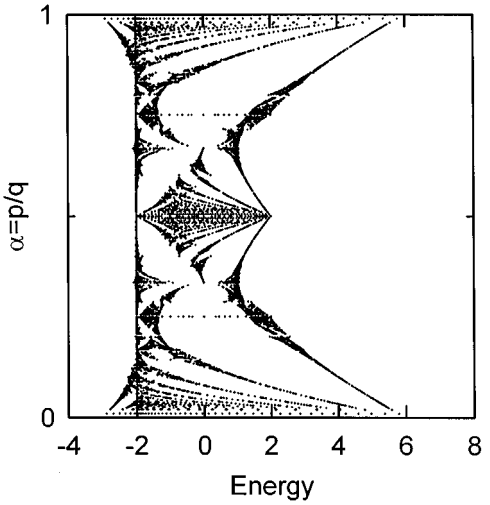

FIG. 1. The energy E/t_+ (in units of E_0) of a hexagonal lattice in a perpendicular magnetic field as a function of the rational flux quantum $\alpha=p/q$. The parameters used in the calculation are $t_0=t_-=t_+=1$. The wave vector is chosen with $k_x=0$, $k_y=0$.

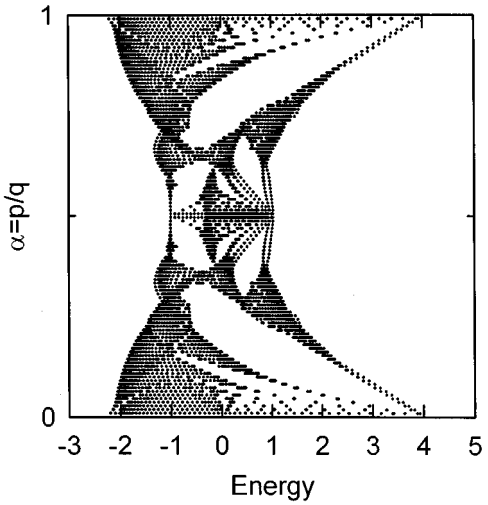

FIG. 2. The same as Fig. 1, except that $t_0=1$, $t_-=1$, $t_+=2$.

nth Landau subband for a square lattice. Neumann and Rauh[23] included second-order terms in a perturbation treatment of the Landau eigenstates to obtain the broadening of the lowest Landau levels due to a square lattice. Making use of Landau eigenstates, Wannier[24] demonstrated the existence of nesting structures in the electron energy spectrum, thereby discovering a possible link between the results of this approach and Bloch electrons in a magnetic field. Kuhn *et al.*[25] have described the effect of including higher Fourier terms of the crystal potential on the electron energy spectrum and have related their results to those obtained with second-nearest-neighbor coupling in the tight-binding approximation. More recent contributors to the field[26–31] have calculated the energy spectrum of a 2D ES in the presence of a spatially modulated magnetic field or a combined constant magnetic field and a spatially modulated perpendicular magnetic field commensurate with the lattice.

For magnetic fields of intermediate strength, i.e., when the magnetic field and the lattice potential are comparable, one should include Landau level coupling. Petschel and Geisel[32] have obtained a generalization of the Harper equation in the vector form by employing a Landau basis and concluded that interband coupling removes the symmetry in the butterfly spectrum. The role played by Landau level coupling has also been determined by Kuhn, Selbmann, Fessatidis, and Cui[16] for 2D electrons in a 2D square array of scatters for various potential strengths and the steepness of the potential profile.

The rest of this paper is organized as follows. In Sec. II, we describe the model used and derive the Schrödinger equation in matrix form. Section III is devoted to numerical results and discussion. In Sec. IV, we present a summary of our results.

II. GENERAL FORMULATION OF THE PROBLEM

For a 2D lattice with hexagonal symmetry, it can be shown that in the absence of an external magnetic field, the lowest energy band with anisotrpic nearest-neighbor overlap is given by[33]

$$E=2E_0\{t_0\cos(k_xa)+t_+\cos[(k_x+k_y\sqrt{3})a/2] +t_-\cos[(k_x-k_y\sqrt{3})a/2]\}, \tag{1}$$

where a is the lattice constant and the atom at the origin has nearest neighbors $(\pm a,0)$ and $(\pm a/2,\pm\sqrt{3}a/2)$, and $\mathbf{k}=(k_x,k_y)$ is the wave vector of an electron. In this notation, t_0 is the nearest-neighbor overlap in the x direction and $t_\pm$ are the nearest-neighbor overlap integrals along the symmetry directions which make $\pi/3$ and $2\pi/3$ with this direction. E_0 is an energy scale related to the bandwidth. We now use the Peierls substitution to construct the Hamiltonian by replacing the Bloch wave vector by the momentum operator in the following way, i.e., $\hbar\mathbf{k}\rightarrow\mathbf{p}+e\mathbf{A}$, where the vector potential is chosen in the Landau gauge with $\mathbf{A}=(0,Bx,0)$, for a constant magnetic field B in the z direction.

Expressing all energies in units of E_0, denoting the wave function by $\psi(x,y)$ and noting that the nearest-neighbor coordinates are $x=ma/2$ $(m=\pm1,\pm2)$ and $y=na\sqrt{3}/2$ $(n=0,\pm1)$, the time-independent Hamiltonian is given by

$$\begin{aligned}\mathcal{H}\psi(mb,nb\sqrt{3})=&\,t_0\{\psi[(m-2)b,nb\sqrt{3}]+\psi[(m+2)b,nb\sqrt{3}]\}\\&+t_+[\psi[(m-1)b,(n-1)b\sqrt{3}]e^{ieBxb\sqrt{3}/\hbar}+\psi[(m+1)b,(n+1)b\sqrt{3}]e^{-ieBxb\sqrt{3}/\hbar}]\\&+t_-[\psi[(m-1)b,(n+1)b\sqrt{3}]e^{-ieBxb\sqrt{3}/\hbar}+\psi[(m+1)b,(n-1)b\sqrt{3}]e^{ieBxb\sqrt{3}/\hbar}],\end{aligned} \tag{2}$$

where, for convenience, we have set $b=a/2$. In what follows, we can assume a plane wave-like behavior in the y direction[5] with $\psi(mb,nb\sqrt{3})=\exp(ink_ya)G(m)$. Equation (2) is further simplified by replacing x in the exponential by $ma=2mb$ so that the argument of the exponent is

$$\Gamma_m=\frac{2mb^2\sqrt{3}eB}{\hbar}=\frac{2\pi mBA_c}{\phi_0}, \tag{3}$$

where $A_c=2b^2\sqrt{3}$ is the area of a unit cell and $\phi_0=h/e$ is the flux quantum. Our numerical results will be restricted to the case when the flux through a unit cell BA_c is a rational fraction $\alpha=p/q$ of the flux quantum. The energy eigenvalues E are then obtained as solutions of the Schrödinger equation

$$\begin{aligned}EG(m)=t_0[G(m-2)+G(m+2)]+[t_+e^{i(2\pi m\alpha-k_ya)}+t_-e^{-i(2\pi m\alpha-k_ya)}]G(m-1)\\+[t_-e^{i(2\pi m\alpha-k_ya)}+t_+e^{-i(2\pi m\alpha-k_ya)}]G(m+1),\end{aligned} \tag{4}$$

where m is to be set successively to $m=1,2,\ldots,q$ since the set of equations are repeated for $m\geq q+1$. Equation (4) is a generalization of Harper's equation for the hexagonal lattice. We use the Bloch condition for the wave function and take

$$\begin{aligned}G(-1)=e^{-ik_xqa}G(q-1),\quad G(0)=e^{-ik_xqa}G(q),\\G(q+1)=e^{ik_xqa}G(1),\quad G(q+2)=e^{ik_xqa}G(2),\end{aligned} \tag{5}$$

which then give the following matrix which must be diagonalized to obtain the energy eigenvalues E/t_+:

$$\vec{A}=\begin{pmatrix}
0 & \Delta_1 & t_0/t_+ & 0 & 0 & \cdots & 0 & (t_0/t_+)e^{-ik_xqa} & \Delta_1^*e^{-ik_xqa}\\
\Delta_2^* & 0 & \Delta_2 & t_0/t_+ & 0 & \cdots & 0 & 0 & (t_0/t_+)e^{-ik_xqa}\\
t_0/t_+ & \Delta_3^* & 0 & \Delta_3 & t_0/t_+ & \cdots & 0 & 0 & 0\\
0 & t_0/t_+ & \Delta_4^* & 0 & \Delta_4 & \cdots & 0 & 0 & 0\\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots\\
0 & 0 & 0 & 0 & 0 & \cdots & 0 & \Delta_{q-2} & t_0/t_+\\
(t_0/t_+)e^{ik_xqa} & 0 & 0 & 0 & 0 & \cdots & \Delta_{q-1}^* & 0 & \Delta_{q-1}\\
\Delta_qe^{ik_xqa} & (t_0/t_+)e^{ik_xqa} & 0 & 0 & 0 & \cdots & t_0/t_+ & \Delta_q^* & 0
\end{pmatrix}, \tag{6}$$

where

$$\Delta_m\equiv(t_-/t_+)e^{i[2\pi m(p/q)-k_ya]}+e^{-i[2\pi m(p/q)-k_ya]}. \tag{7}$$

III. NUMERICAL RESULTS AND DISCUSSION

We now present our results for the Hofstadter-type energy spectrum for a 2D hexagonal lattice in a perpendicular magnetic field. The commensurability between the lattice and magnetic Brillouin zones again leads to an interesting Bloch band splitting and symmetry patterns which were obtained for the square lattices in the two limiting regimes discussed above: Bloch electrons in a weak uniform magnetic field and Landau quantized electrons in a weak 2D lattice potential. The energy spectrum we obtain applies only to rational values of α for the magnetic flux through a unit cell. For a chosen value of q, there are as many energy eigenvalues obtained by diagonalizing the matrix in Eq. (6). However,

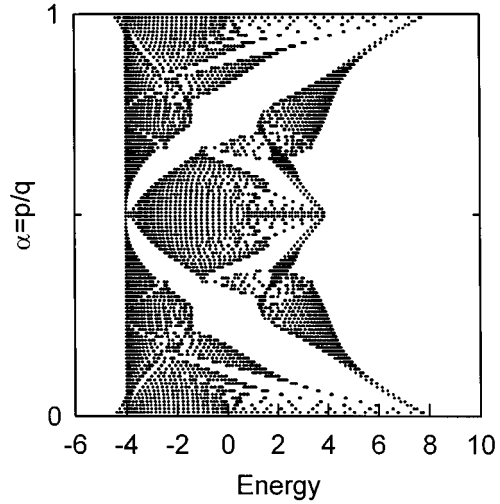

FIG. 3. The same as Fig. 1, except that $t_0=2$, $t_-=1$, $t_+=1$.

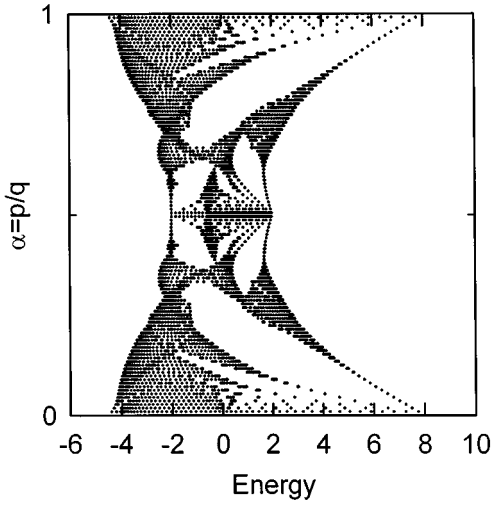

FIG. 4. The same as Fig. 1, except that $t_0=1$, $t_-=2$, $t_+=1$.

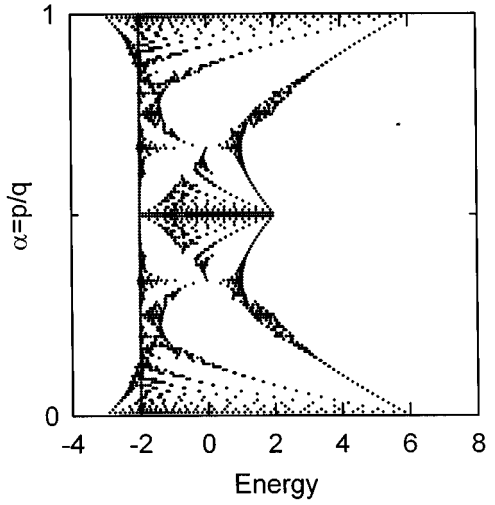

FIG. 5. The same as Fig. 1, except that $k_x=\pi/2$, $k_y=0$.

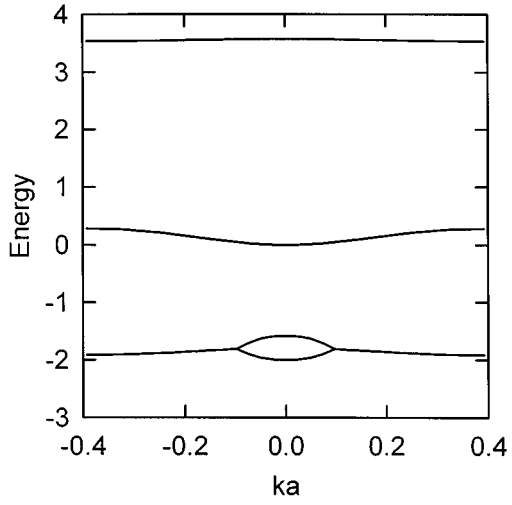

FIG. 6. The energy dispersion as a function of k_xa for $k_y=0$, $t_0=t_-=t_+=1$, and $\alpha=p/q$, with $p=1$ and $q=8$.

our numerical calculations have shown that the energy eigenvalues are highly degenerate (there is double and quadruple degeneracy) for a chosen value of the wave vector **k**. As a consequence, the resulting eigenvalue spectrum is not symmetric about the middle of the band as it is for a square lattice. We follow Hofstadter,[5] Hasewaga *et al.*,[15] and Gumbs *et al.*,[28] and plot the energy versus α to make a comparison with the square, triangular, and honeycomb lattices. Since the energy spectrum is periodic in $1/\alpha$, Claro and Wannier,[14] Kuhn *et al.*,[17] and Gerhardts *et al.*[31] presented their results for the energy as a function of the inverse of this rational fraction of the flux since they included several Landau subbands and intersubband coupling.

Figure 1 is the energy spectrum resulting from the numerical diagonalization of Eq. (6); the overlap integrals are chosen as $t_0=t_-=t_+=1$ and the wave vector **k** is at the center of the magnetic Brillouin zone. Since the energy eigenvalues are highly degenerate, the spectrum lacks the symmetry about the middle of the band which is present in the Hofstadter ''butterfly'' for a square lattice. However, there is symmetry about $\alpha=1/2$ and clustering patterns are still obtained. Furthermore, energy gaps which are characteristic of the Hofstadter butterfly are also present in the fractal patterns. There is a distinct array of energy eigenvalues parallel to the energy axis in the two largest energy gaps. The overall pattern in Fig. 1 of this paper is similar to, but not identical with Fig. 1 in the paper by Claro and Wannier[14] which was obtained using free-electron Landau eigenfunctions as a basis set and diagonalizing the resulting matrix.

In Fig. 2, we present results for the energy as a function of α for $t_0=t_-=1$ and $t_+=2$ with the wave vector $\mathbf{k}=\mathbf{0}$. Comparing these results with Fig. 1, we still have a fractal structure. However, the distinct array of eigenvalues parallel to the energy axis in the two largest energy gaps are not present and there is a larger degree of degeneracy and a broadening of the energy band.

For Fig. 3, we chose $t_0=2$ and $t_+=t_-=1$ with the wave vector still at the center of the magnetic Brillouin zone. For this choice of values of the overlap integrals, some of the degeneracy is lifted for a chosen value of q. The bottom of the band is very flat near $E=-4$ and the eigenvalue spectrum is symmetric about $\alpha=1/2$.

We have chosen $t_0=t_+=1$ and $t_-=2$ in Fig. 4 still keeping $\mathbf{k}=\mathbf{0}$. These values for the overlap integrals result in a broadening of the energy band in Fig. 2 for which the values of t_- and t_+ are interchanged but all the values for t_0 and the wave vector remain the same. One difference between Figs. 2 and 4 is the absence of the two sets of horizontal eigenvalues within the largest energy gaps in Fig. 2 which are now replaced by a single string of energy eigenvalues.

Figure 5 presents the energy spectrum for the same values of t_0, t_-, t_+ as in Fig. 1, except that a finite value of the wave vector is chosen with $k_xa=\pi/2$ and $k_y=0$. The degeneracy of the energy eigenvalues obtained from diagonalizing Eq. (6) is greatly increased. These results show the wave vector dependence of the energies should be further explored. For this, we show the dispersion relation in Fig. 6 for $p=1$ and $q=8$. For $q=8$, Eq. (6) gives eight eigenvalues. However, for $-1\lesssim k_xa\lesssim 1$ there are four eigenvalues each of which is doubly degenerate. For $k_xa\gtrsim 1$, the two highest eigenvalues remain doubly degenerate while the lowest subband is fourfold degenerate.

IV. CONCLUDING REMARKS AND SUMMARY

In this paper, we have presented a theoretical formulation and numerical results for the eigenvalue spectrum of a 2D ES in the tight-binding approximation for a lateral surface superlattice with hexagonal symmetry in a uniform perpendicular magnetic field. Our results show a clustering pattern and energy gaps like the Hofstadter butterfly, except that for zero wave vector there is no symmetry about the middle of the energy band as for a square lattice. The eigenvalues are highly degenerate compared to the square lattice and this degeneracy increases at finite wave vector.

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*Also at The Graduate School and University Center of the City University of New York, 33 West 42 Street, New York, NY 10036.

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