Electron hopping in three-dimensional flux states

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We point out that the eigenvalue problem of an electron hopping on a lattice with arbitrarily oriented three-dimensional flux states can be reduced to a one-dimensional hopping in a suitably chosen gauge. The energy spectra and the density of states are calculated for various flux states. In general, overlapping energy bands are found. In special configurations the bands touch each other (zero gap). Where the bands touch the density of states vanishes. The energy spectrum is calculated for flux states of orientation $(2\pi p/q, 2\pi p/q, 2\pi p/q)$ and $(\pi,\pi,2\pi p/q)$ for all rational values with $q<38$ and <30, respectively. The spectra have some traces of the properties of the two-dimensional model. When the center of the energy band is plotted as a function of p/q a "butterfly" pattern reminiscent of Hofstadter's butterfly emerges. In many cases, the total energy of electrons can be lowered by applying an appropriate uniform magnetic field.

I. INTRODUCTION

Fifteen years ago, Hofstadter,[1] expanding upon earlier work by Azbel,[2] astonished the physics community by showing that the problem of an electron hopping on a lattice in a uniform magnetic field has a rich and intricate structure. The relevant Hamiltonian is simply

$$\mathcal{H}=\sum_i (U_{ix}c^\dagger_{i+x}c_i+U_{iy}c^\dagger_{i+y}c_i+\text{H.c.}) , \tag{1.1}$$

where c_i and $c_i^\dagger$ are the annihilation and creation operators on the site $i=(i_x,i_y)$, respectively. The magnetic flux Φ through the plaquette is defined by

$$e^{i\Phi}=\prod_{\substack{\text{square}\\ \text{plaquette}}} U , \tag{1.2}$$

where the right-hand side represents the product of the U's around a plaquette. By a gauge choice, we can set $U_{iy}=1$. The choice

$$U_{ix}=e^{i2\pi(p/q)i_y} \tag{1.3}$$

corresponds to $\Phi=2\pi(p/q)$. Henceforth we will measure Φ in units of 2π and write $\Phi=2\pi\phi$. The problem is solved by going to momentum space,

$$H=\sum_k (c^\dagger_{k+w}c_k e^{ik_x}+c^\dagger_k c_k e^{ik_y}+\text{H.c.}) , \tag{1.4}$$

where $w=(0,2\pi p/q)$. Thus we obtain a one-dimensional hopping problem in which a particle hops from k to $k+w$, to $k+2w$, and so on. For p and q incommensurate integers, the problem closes: After q hops in a given direction, the particle returns to its original site in momentum space. The energy eigenvalues of $\mathcal{H}$ are thus determined by diagonalizing a $q\times q$ matrix. There are thus q bands. We can easily see why the problem has a rich structure such that a physicist used to thinking in continuum terms would find amazing. For instance, the fluxes $\phi=\frac{1}{2}$ and $\frac{43}{99}$, while numerically close to each other, produce a drastically different energy spectrum.

All of this is, of course, exceedingly well known by now and has been extensively studied. For instance, index theorems may be proved showing that there exist[3,4] q Dirac zeros for $\phi=p/q$. In recent years the Hofstadter problem has assumed great importance[5–7] in connection with the quantum Hall effect. More recently, it has formed the basis for a number of speculative ideas regarding the ground state of strongly correlated electron system and a possible theory of high-temperature superconductivity. Thus the flux state,[8] the chiral spin state,[9] and the commensurate flux state,[10] among others, have all been studied as possible ground states. Within the last year or so, various authors[11–15] have ventured forward and studied the Hofstadter problem suitably generalized to three dimensions. We will follow in particular the work of Hasegawa.[14] The motivations for moving to three dimensions are given as follows: (1) There may be a quantized Hall effect in three dimensions. (2) Interlayer effects may be important in high-temperature superconductors. (3) The appearance of the Dirac zero may be relevant for particle physics. Let us admit, however, that at this point, the main motivation may still be simply exploratory.

The Hamiltonian (1.1) is easily extended to three dimensions:

$$\mathcal{H}=\sum_i t_x c^\dagger_{i+x}U_{ix}c_i+t_y c^\dagger_{i+y}U_{ij}c_i+t_z c^\dagger_{i+z}U_{iz}c_i+\text{H.c.} \tag{1.5}$$

In general, of course, it is possible to have different hopping amplitudes t_x,t_y,t_z in the three orientations. Unless we specify otherwise, we will generally take $t_x=t_y=t_z=1$.

II. REDUCTION TO ONE-DIMENSIONAL HOPPING

We wish to study the energy spectrum when the lattice is pierced by flux ϕ_x in the x direction, ϕ_y in the y direction, and ϕ_z in the z direction. We will label a flux arrangement by (ϕ_x,ϕ_y,ϕ_z). By a gauge choice, we can always set U_{iy}, say, to 1. It would thus appear that the three-dimensional problem would reduce in momentum space to a two-dimensional hopping problem. Thus, for instance, in Ref. 13 the choice

$$U_{ix}=e^{-ici_y}e^{ibi_x},\quad U_{iy}=1,\quad U_{iz}=e^{iai_y} \tag{2.1}$$

was made. This corresponds to the flux arrangement $(\phi_x,\phi_y,\phi_z)=(a,b,c)/(2\pi)$. The position dependence of the U's is such that clearly in momentum space a particle at k may in one hop get to either $k\pm u$ or $k\pm w$ with the vectors $u=(0,-c,b)$ or $w=(0,a,0)$. The equivalent hopping problem is two dimensional.

Recently Hasegawa[14] has studied the flux arrangements $(0,\phi,\phi)$ and (ϕ,ϕ,ϕ) for certain selected values of ϕ. For (ϕ,ϕ,ϕ), that is, for the special case in which ϕ_x, ϕ_y, and ϕ_z are all equal, he found a clever gauge choice which again reduces the problem to a one-dimensional hopping problem in momentum space.

The basis of this paper is the realization that in fact even in the general case of unequal ϕ_x, ϕ_y, and ϕ_z there exists a gauge choice such that we still have a one-dimensional hopping problem in momentum space. We find this result remarkable in that it renders the three-dimensional Hofstadter problem only slightly more involved that the two-dimensional problem. The idea is simply to rotate the vector w until it is parallel to u. We can do this by replacing U_{iz} in (2.1) by

$$U_{iz}=e^{iai_y}e^{-idi_z}\ . \tag{2.1'}$$

It is easy to see that this does not affect the flux at all. (For instance, consider the product of the U's around a plaquette in the y-z plane.) The factor e^{-idi_z} cancels itself "coming and going." More formally, the U_{iz} in (2.1') is related to the old U_{iz} in (2.1) by the gauge transformation $U_{iz}=W^*_{i+z}U^{\rm old}_{iz}W_i$ with $W_i=e^{idi_z(i_z-1)/2}$. The vector w now becomes $w=(0,a,-d)$. If we choose the ratio d to b such that

$$d/b=a/c\ , \tag{2.2}$$

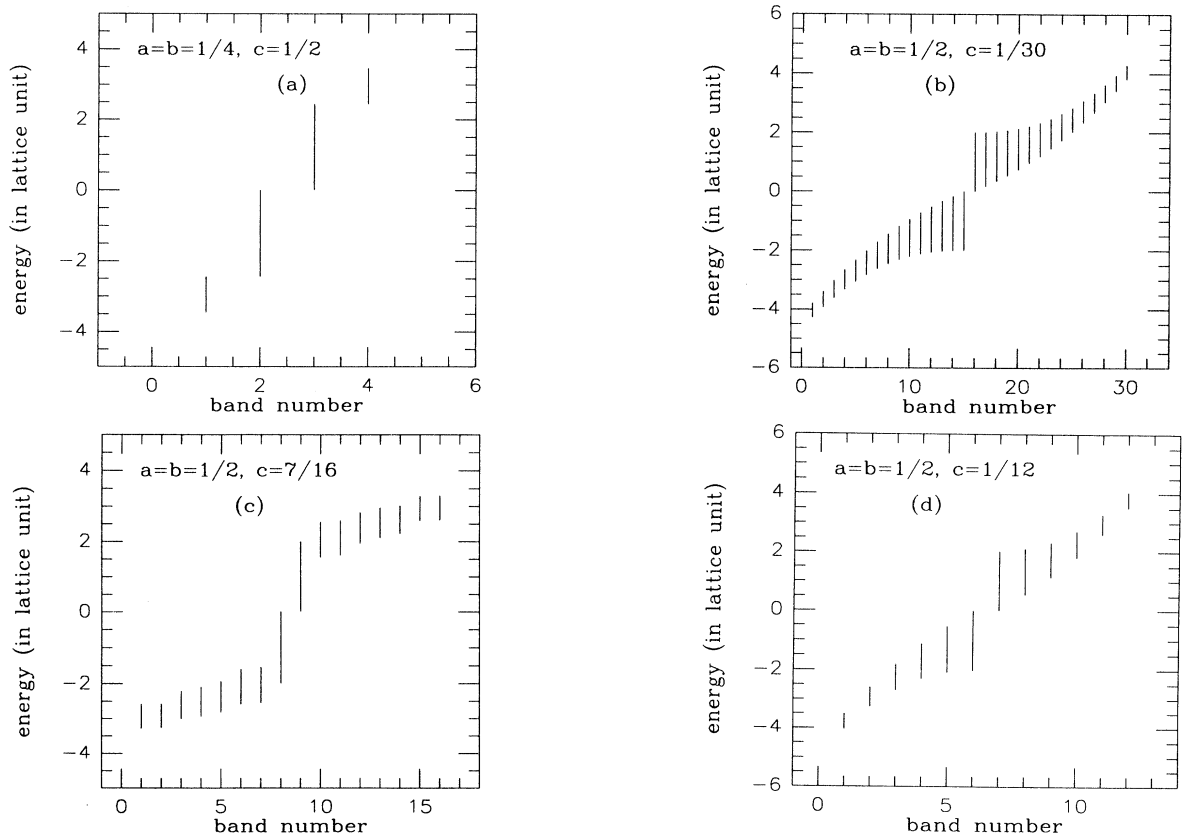

FIG. 1. Energy bands plotted vs the band number for four different flux states: (a) $(\frac{1}{2},\frac{1}{4},\frac{1}{4})$, (b) $(\frac{1}{2},\frac{1}{2},\frac{1}{30})$, (c) $(\frac{1}{2},\frac{1}{2},\frac{7}{16})$, and (d) $(\frac{1}{2},\frac{1}{2},\frac{1}{12})$.

then w is parallel to $u=(0,-c,b)$. This is now a one-dimensional hopping problem, although with non-nearest-neighbor hops. (In fact, with $a=c$, that is, with two of the fluxes ϕ_x, ϕ_y, and ϕ_z equal, we still have only nearest-neighbor hops.) Thus, for instance, for $(\phi_x,\phi_y,\phi_z)=(\frac{1}{2},\frac{1}{3},\frac{1}{4})$, $u=2\pi(0,-\frac{1}{4},\frac{1}{3})$, and $w=2\pi(0,\frac{1}{2},-\frac{2}{3})=2u$. After 12 hops, the particle is back to where it was. In contrast to the original Hofstadter problem, the particle is now allowed to do a "double hop," jumping either one site or two sites at a time.

In general, the energy eigenvalues are given by the equation

$$\psi(k+u)e^{ik_x}+\psi(k-u)e^{-ik_x}+\psi(k)(2\cos k_y-E)+\psi(k+w)e^{ik_z}+\psi(k-w)e^{-i(k-w)_z}=0\ , \quad (2.3)$$

where u and w are integral multiples of each other. For $(\phi_x,\phi_y,\phi_z)=(p_x/q_x,p_y/q_y,p_z/q_z)$, the number of sites on the hopping circle is given by the lowest common denominator of the three fractions.

We are thus able to study the general case of unequal ϕ_x,ϕ_y,ϕ_z not studied by Hasegawa. We would like to see, for instance, how the many interesting results[14] obtained by Hasegawa for (ϕ,ϕ,ϕ) may be modified by moving away slightly from the equal-flux arrangement. We would also like to study what happens when the three fluxes are not close to each other in numerical value.

III. ENERGY SPECTRUM

In simple cases the energy spectrum of Eq. (2.2) can be solved analytically. For example, for $(a,b,c)=(\frac{1}{4},\frac{1}{4},\frac{1}{2})$, the spectrum is given by the solution of the equation

$$E^4-12E^2+6-3\cos 4k_x-3\cos 4k_y-3\cos 4k_z-16\sin^2 k_y\sin^2 k_z-16\cos^2 k_y\cos^2 k_z+32\cos k_x\sin k_y\cos(k_z+k_y)=0\ , \quad (3.1)$$

which gives four energy bands [see Fig. 1(a)]. Each of the bands touches the one directly above it (i.e., there is no gap), and they are symmetric around $E=0$:

$$E=(-2\sqrt{3},-\sqrt{6}),(-\sqrt{6},0),(0,\sqrt{6}),(\sqrt{6},2\sqrt{3})\ , \quad (3.2)$$

where the notation (E_-,E_+) indicates that the band

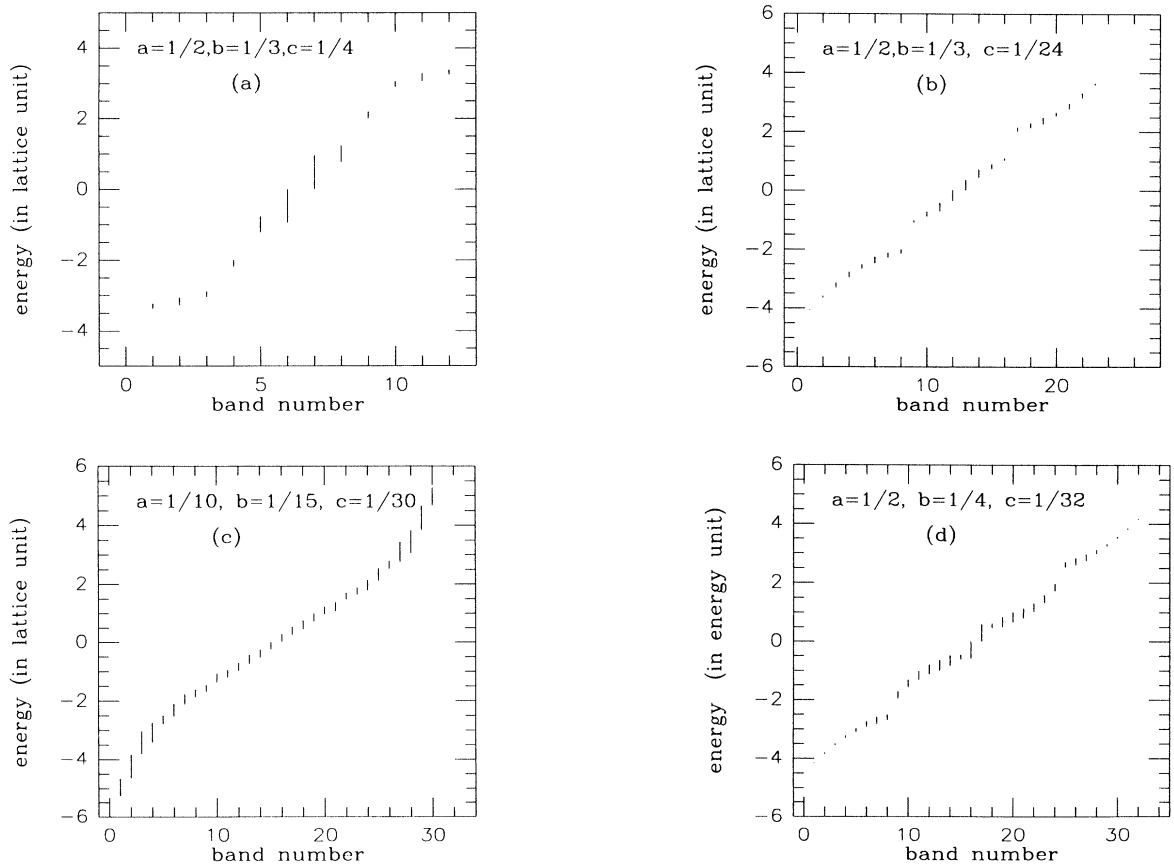

FIG. 2. The same as Fig. 1, but for (a) $(\frac{1}{2},\frac{1}{3},\frac{1}{4})$, (b) $(\frac{1}{2},\frac{1}{3},\frac{1}{24})$, (c) $(\frac{1}{10},\frac{1}{15},\frac{1}{30})$, and (d) $(\frac{1}{2},\frac{1}{4},\frac{1}{32})$.

runs from E_- to E_+. We reach the edges of the band at $k_x=-k_y=k_z=\pi/4$. If we expand around the zero-energy state in the long-distance limit, we again get the Dirac equation. It would be interesting to generalize the theorem proved for the two-dimensional case,[3,4] which would relate the number of Dirac zeros to the flux values.

As another example, consider the case $(\frac{1}{2},\frac{1}{2},\frac{1}{30})$, which is rather close to the value $(\frac{1}{2},\frac{1}{2},0)$. In the latter case the spectrum consists of two bands which touch each other at zero energy: $(-2\sqrt{5},0)$ and $(0,2\sqrt{5})$. If now we change slightly the flux component from zero to $\frac{1}{30}$ in the z direction, we obtain 30 bands symmetric around $E=0$. The bands all overlap except at $E=0$ when they touch each other [see Fig. 1(b)]. The bandwidths are smaller and the maximal energy is smaller then in the $(\frac{1}{2},\frac{1}{2},0)$ case. It is amusing to compare the energy bands obtained for $(\frac{1}{2},\frac{1}{2},\frac{1}{30})$ and $(\frac{1}{2},\frac{1}{2},\frac{7}{16})$ plotted in Figs. 1(b) and 1(c). The centers of the band show a rather different distribution. Further illustrative examples are shown in Figs. 1(d) and 2(a)–2(d).

We can see in Figs. 1(a)–1(d) and 2(a)–2(d) that, contrary to the two-dimensional case, the energy bands can overlap or touch each other. We cannot, however, exclude the existence of gaps in a general flux state [see Figs. 2(a)–2(d)].

With numerical diagonalization of the eigenvalue matrix of Eq. (2.2), we can easily find the spectrum for arbitrary flux states. The computer time available limits ultimately the maximal value of q we can consider. In Figs. 3(a) and 3(b) we plot the center of the bands as a function of p/q for symmetric flux states of the form $(p/q,p/q,p/q)$ and for $(\frac{1}{2},\frac{1}{2},p/q)$ at all values p/q with $q<38$ and $q<30$, respectively. It is remarkable that for magnetic fields along the main diagonal of the cubic cell in three dimensions the centers of the bands give the same butterfly patterns in the energy-flux plane as the pattern of the energy bands found by Hofstadter in the two-dimensional (2D) case. The spectrum of the three-dimensional model in this case is closely related to the spectrum of the two-dimensional model. It is interesting to compare the patterns shown in Figs. 3(a) and 3(b). In the more asymmetric case $(\frac{1}{2},\frac{1}{2},p/q)$, a gap appears around zero energy, but in the remaining part of the plot the usual pattern appears again. This reflects the fact that in this case the lowest bands are broader than 2×1.142.

A striking feature of the clustering of the energy bands in the 2D case[1] is its self-similarity. It is visually suggestive from Figs. 3(a) and 3(b) that the same self-similarity pattern may remain valid also in the 3D case. Although an exhaustive numerical study of this question would be interesting, we restrict ourselves here only to a few comments.

For the patterns given in Figs. 3(a) and 3(b) following Hofstadter[1] we can define the skeleton of the graph and we can introduce the concept of R and L subcells given by the trapezoidal boxes above and below the gaps between the "pure" values $1/N$ and $1/(N+1)$, where $N\gtrsim2$. For the central parts one can again define the C subcells. For the $L_{\pm N}$ and $R_{\pm N}$ subcells following Hof-

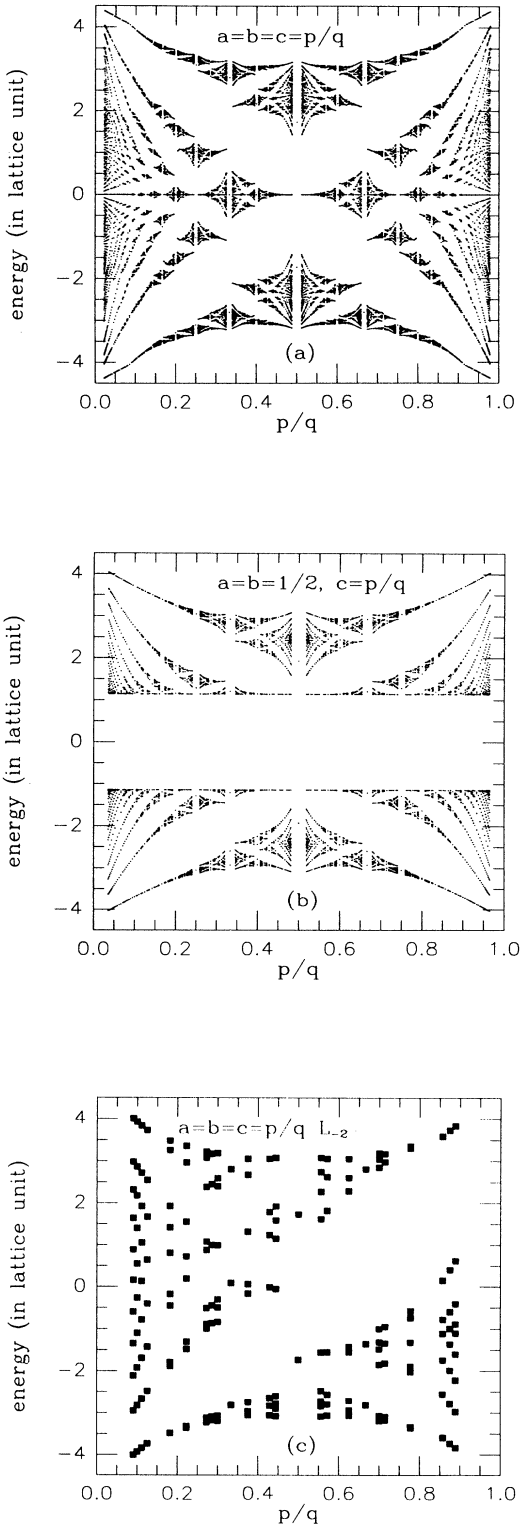

FIG. 3. Centrum of the energy bands for flux states (a) $(p/q,p/q,p/q)$ for $q<38$ and (b) $(\frac{1}{2},\frac{1}{2},p/q)$ for $q<30$ as a function of p/q; (c) the L_{-2} subcell plotted in terms of local coordinates after linear stretching (see text).

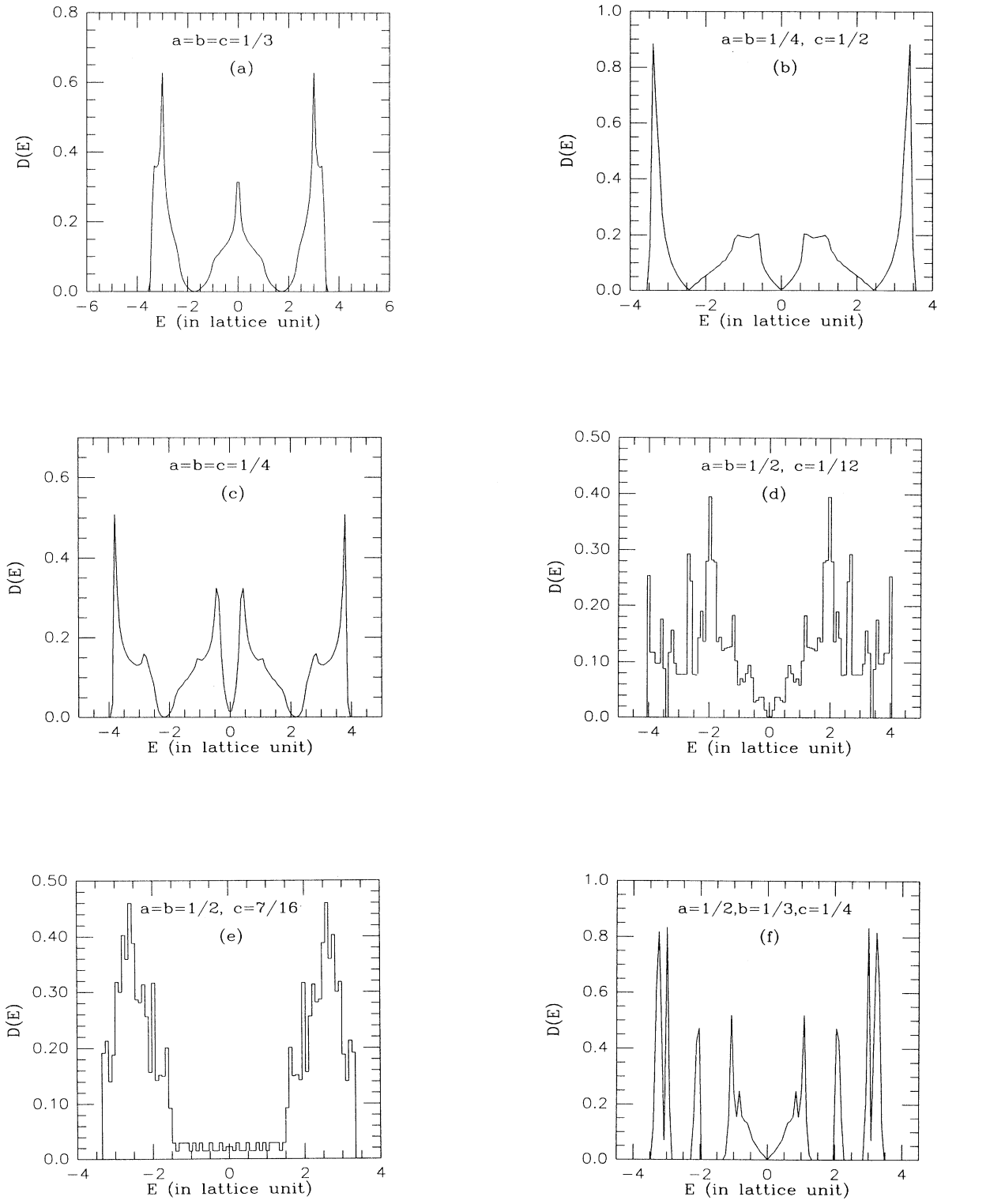

FIG. 4. Density of states as a function of the energy for seven different flux states: (a) $(\frac{1}{3},\frac{1}{3},\frac{1}{3})$, (b) $(\frac{1}{4},\frac{1}{4},\frac{1}{2})$, (c) $(\frac{1}{4},\frac{1}{4},\frac{1}{4})$, (d) $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$, (e) $(\frac{1}{2},\frac{1}{2},\frac{7}{16})$, (f) $(\frac{1}{2},\frac{1}{3},\frac{1}{4})$, and (g) $(\frac{1}{10},\frac{1}{15},\frac{1}{30})$. The densities have been collected in bins with the Monte Carlo method, and the histogram values are plotted either connecting the values at the centers of the bins or as histograms. The numerical evaluation has about 1% accuracy.

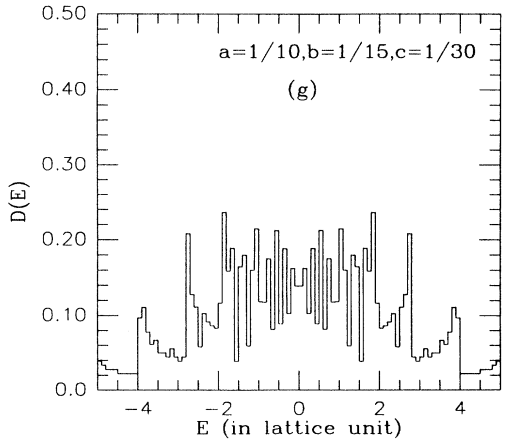

FIG. 4. (*Continued*).

stadter, we introduce the local variables

$$p'/q' = q/p - N, \quad N \gtrsim 2 , \tag{3.3}$$

which maps the subcell into a unit cell. If q and p are relative primes, then also p' and q' are relative primes. Therefore, $p' = q - Np$ and $q' = p$. The local variables of a C subcell are given by the equation

$$\tilde{p}/\tilde{q} = \left\lfloor \frac{p}{q-2p} \right\rfloor , \tag{3.4}$$

and therefore,

$$\tilde{q} = q - 2q' . \tag{3.5}$$

The division into subcells naturally given by the large four gaps appearing in the butterfly pattern splits the bands into three groups, and we have found from our numerical analysis that it is an inherent property of the spectrum given in Figs. 3(a) and 3(b) that the number of the bands in these three groups at a given value of p/q precisely matches the values required by the local coordinates:

$$q' - \tilde{q} - q' . \tag{3.6}$$

We conclude that the clustering property of the energy bands found by Hofstadter in two dimensions remains valid also in three dimensions at least for cubic cell diagonal [Fig. 3(a)] flux states. This leads to a recursive breakdown of the graphs of Fig. 3(a). A similar recursive breakdown can also be established for the plain diagonal case [Fig. 3(b)].

In the 2D case Hofstadter found a "nearly" isomorphic map of the subcells into the unit cell with a *linear stretching (rectangularization)* at each local height, making the effective width of the subcells the same as the width at the same height of the initial unit cell. The result of such

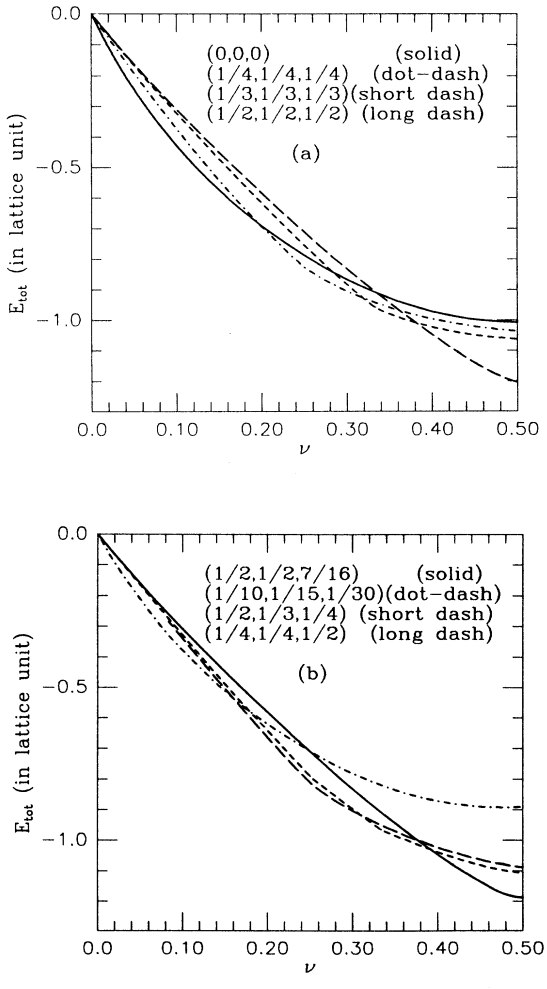

FIG. 5. Total energy of the electrons as function of the electron filling ν (a) for flux states (0,0,0), $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$, $(\frac{1}{3},\frac{1}{3},\frac{1}{3})$, and $(\frac{1}{4},\frac{1}{4},\frac{1}{4})$, and (b) for flux states $(\frac{1}{2},\frac{1}{3},\frac{1}{4})$, $(\frac{1}{2},\frac{1}{2},\frac{7}{16})$, $(\frac{1}{2},\frac{1}{4},\frac{1}{4})$, and $(\frac{1}{10},\frac{1}{15},\frac{1}{30})$.

a simple linear map of the subcell L_{-2} [it is given by the centers of the energy bands of Fig. 3(a) with $E_c < -2$ at heights $\frac{1}{4} \lesssim p/q \lesssim \frac{1}{3}$] are plotted as a function of the local variables p'/q'. We can see that in three dimensions such a simple map is not able to reproduce precisely the starting pattern [see Fig. 3(c)]. The symmetry for positive and negative energies and the mirror symmetry through the axis $p/q = \frac{1}{2}$ are not yet restored. Since the number of the points at a given height in all the subcells are the same as the corresponding number in the initial unit cell, the existence of such a simple linear map is not crucial for the recursive breakdown of the graph.

We also investigated the density of states in various flux states. We reproduced the distributions found by Hasegawa and calculated the densities in the more general case of nonequal values of a, b, and c [see Figs. 4(a)–4(g)].

Investigating only configurations of the form $(0,0,\phi)$, $(0,\phi,\phi)$, and (ϕ,ϕ,ϕ), Hasegawa found that the total energy of the electrons can be lowered with respect to the vacuum configuration. With our study of the general configurations, we confirm Hasegawa's result that the minimum value of the total energy, at the commensurate filling $\nu=\phi$, is obtained for a magnetic field directed along the main diagonal of the cubic cell (ϕ,ϕ,ϕ) provided $\phi \gtrsim \frac{1}{8}$. The minimal energy is obtained for $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ with half-filling. In Figs. 5(a) and 5(b) we have plotted the total energy of the electrons as a function of the filling factor for various flux states in order to illustrate the emergence of Hasegawa's result.

IV. SUMMARY

We have made an exploratory study of an electron hopping on a three-dimensional lattice in an arbitrarily oriented external magnetic flux. We have pointed out that the problem can be reduced to a one-dimensional hopping problem in momentum space with a suitable gauge choice. Contrary to the two-dimensional case, there is no gap in the spectrum in the three-dimensional case. If a field $(p/q,p/q,p/q)$ is applied in the [111] direction, the energy spectrum has a remarkable trace of the two-dimensional case: The distribution of the centers of the energy bands in the energy-flux plane shows a pattern similar to the butterfly pattern of the energy bands of the two-dimensional case [Fig. 3(a)]. If the field is tilted between the main and plain diagonal directions keeping the magnetic flux ϕ_x,ϕ_y fixed $(\frac{1}{2},\frac{1}{2})$, for the centers of the bands there is a forbidden region around zero energy. The trace of the two-dimensional structure can also be seen in the density of states[14] as zeros at some energy values. Investigating numerous examples of general field orientations, we confirm the result of Hasegawa that the lowest-energy state is obtained for flux state $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ with half-filling.

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