Magnetic subband structure of electrons in hexagonal lattices

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The energy spectrum of an electron in the presence of a uniform magnetic field and a potential of hexagonal symmetry is analyzed. Two alternative approaches are used, one that takes as a basis set free-electron Landau functions, and a second one that treats an effective single-band Hamiltonian with the Peierls substitution. Both methods lead to consistent results. The energy spectrum is found to have recursive properties similar to those discussed by Hofstadter for the case of a square lattice. The density of states over each subband of the spectrum has the same structure as that for the original field-free band. The plot of integrated density of states versus field is also discussed.

I. INTRODUCTION

Over the past two decades the magnetic field has been used extensively as a probe for the electronic properties of solids. The understanding of the ensuing effects has been based on the picture that for sufficiently high fields the conduction electrons are clustered in Landau states. The lattice potential broadens the levels and changes the effective mass thus making the cyclotron frequency a function of energy. In the language of the semiclassical treatment broadening allows switching between electron orbits and is therefore essential to the understanding of the transport properties in the presence of the field.[1]

Several authors have discussed broadening.[1-6] Chambers suggested that a fine structure could be found within the broadened levels.[3] Langbein showed that the matrix elements between nearly-free-electron states within a level and tight-binding states within a band are given by expressions of the same form if the field parameter is replaced by its inverse in going from one representation to the other.[7] This finding suggests that in a plot of allowed energies versus field the fine structure within an identifiable Landau state and the entire spectrum are closely related to each other. In fact, a detailed numerical study of the spectrum for a simple square-lattice model carried out by Hofstadter showed the spectrum to have recursive properties.[8] In his spectrum the Landau levels near the bottom of the band broaden as the field is increased and exhibit a fine structure which is (nearly) homeomorphic to the entire spectrum. Hofstadter found this homeomorphism to be ingrained in the whole spectrum which led him to postulate a nesting property. This property has not been rigorously proved since the model yields a difference equation for the eigenvalues and our present knowledge of how to handle this kind of equation is limited. It is possible however, that nesting is a property that goes beyond the square-lattice model, as is suggested by the similarity of matrix elements for the internal structure of Landau levels and that of the spectrum as a whole. As we shall show below, nesting is indeed also present if the crystalline potential has hexagonal symmetry. In Sec. II we derive the eigenvalue equation from a basis of Landau functions and discuss broadening and the fine structure of a single Landau level. As pointed out by Obermeir and Wannier[9] this is a convenient approach that uses a set of functions of well-known properties operating in a well-defined Hilbert space. In Sec. III we use the Peierls substitution[10] to obtain for a single-band Hamiltonian the spectrum in the presence of the magnetic field, and discuss nesting. Section IV treats the two-dimensional density of states and Wannier's construction for the integrated density of states as a function of the field.[11]

II. LANDAU-LEVEL FINE STRUCTURE

A straightforward procedure to treat the problem of a charged particle which is acted upon simultaneously by a periodic potential and a magnetic field is to use as a basis set free-electron Landau functions. The crystalline translation group is a subgroup of the magnetic group and the function space in which the basis operates is of well-known properties. Provided that the potential is sufficiently weak the Landau states are still recognizable and the periodic potential just lifts part of their degeneracy. We shall use this procedure in this section.

Let the magnetic field $\vec{H}$ point in the z direction, and let us assume also this direction to be perpendicular to a lattice x-y plane. We choose the Landau gauge $\vec{A}=H(0,x,0)$ for convenience. In this gauge the Landau functions contain as factors a plane wave of wave vector $\vec{k}=(0,k_y,k_z)$ in the y-z plane and a harmonic-oscillator function in

the x coordinate,[12] of index n. In the presence of a lattice potential the motion along the z axis may be separated out in simple cases and for more general potentials a separation scheme such as that proposed by Langbein[7] may be adopted. We shall ignore this feature here and work in two dimensions. The lattice potential then couples degenerate Landau states of different k_y as well as states of different index n. For weak potentials we ignore the latter and obtain for the amplitudes C of degenerate states within the level n, that contribute to an eigenstate of energy E, the matrix equation

$$(E-\epsilon_n)C(k_y)-\sum_{\vec{G}} V_{\vec{G}}\, e^{iG_x(k_y+G_y/2)/\alpha} \times e^{-\vec{G}^2/4\alpha} L_n(\vec{G}^2/2\alpha)C(k_y+G_y)=0\,. \tag{1}$$

This is an adaptation of Eq. (2) of Ref. 9; the value of the matrix element is shown explicitly and the sum over different Landau levels has been suppressed. $V_{\vec{G}}$ is the strength of the Fourier component of reciprocal-lattice vector $\vec{G}=(G_x, G_y, 0)$ of the lattice potential, $\epsilon_n=(\hbar eH/mc)(n+\frac{1}{2})$ is the energy of the free-electron Landau orbit, L_n is a Laguerre polynomial of order n and $\alpha=eH/\hbar c$. We observe that the index k_y in Eq. (1) appears explicitly only in an imaginary exponent; its useful range is therefore limited to a length proportional to the field in reciprocal space. To be specific let the basis vectors on the x-y plane be $\vec{a}$ and $\vec{b}$ and define the dimensionless field parameter

$$\phi=(eH/hc)\,|\vec{a}\times\vec{b}| \tag{2}$$

which measures the number of magnetic-flux quanta traversing a unit cell. One can readily verify then that the imaginary exponent in (1) changes by an integral multiple of 2π if k_y is incremented by $\phi G_y'$ for a rectangular lattice or by $2\phi G_y'$ if the lattice is hexagonal, all G_y'. These increments therefore define the physical range of k_y. The translational symmetry just described can be taken advantage of in practical calculations if the field parameter is a rational number, say, $\phi=q/p$ with q and p integers prime to each other. There is then a particular $G_y'=Q_y$ for which the range of k_y is itself the y component of a reciprocal-lattice vector, and it is just p times the smallest G_y'. The infinite set of equations that result from (1) upon displacement of k_y by all possible G_y' becomes then cyclic and is therefore closed. This property is the basis of recent numerical treatments of the square-lattice case[6-8] and is also used in our treatment of the hexagonal lattice that follows.

In setting up the model, we note that the Gaussian factors in (1) enhance the contribution of the reciprocal-lattice vectors closest to the origin. If we keep only terms nearest to the origin and assume isotropy in the coupling the two-dimensional hexagonal potential has the form

$$V=V_0+2V_1\left[\cos\frac{2\pi}{a}\left(\frac{x}{\sqrt{3}}-y\right)+\cos\frac{4\pi}{a}\frac{x}{\sqrt{3}} +\cos\frac{2\pi}{a}\left(\frac{x}{\sqrt{3}}+y\right)\right], \tag{3}$$

where the y-axis has been chosen in the direction of the basis vector $\vec{b}$. With this potential the set of equations that (1) generates for fixed k_y becomes, after some rearrangement and the use of (2),

$$\lambda C(\kappa+m)=\cos[\pi(\kappa+m-\tfrac{1}{2})/\phi]C(\kappa+m-1) +\cos[2\pi(\kappa+m)/\phi]C(\kappa+m) +\cos[\pi(\kappa+m+\tfrac{1}{2})/\phi]C(\kappa+m+1). \tag{4}$$

Here m may take all integer values, $\kappa=ak_y/2\pi$, and λ is related to the energy through

$$E=\epsilon_n-V_0+2\lambda V_1 e^{-\pi/\sqrt{3}\phi}L_n(2\pi/\sqrt{3}\,\phi)\,. \tag{5}$$

Equation (4) is a second-order difference equation whose bounded solutions determine the broadening and fine structure of the Landau level for a given value of the magnetic field. The spectrum is confined to values of λ between -3 and $+3$. The proof is similar to that given by Rauh for the square lattice.[5] Using these bounds we can estimate the ratio of broadening to the separation between neighboring Landau levels for low n. The result is

$$\frac{\Delta E}{\hbar\omega_c}=\frac{9\sqrt{3}}{\pi}\frac{V_1}{U}\frac{e^{-\pi/\sqrt{3}\phi}}{\phi}L_n\left(\frac{2\pi}{\sqrt{3}\,\phi}\right), \tag{6}$$

where U is the width of the field-free energy band. For $\phi=0.1$ this ratio is of the order of 10^{-7} and becomes smaller for smaller fields.

A close inspection of (4) shows that the spectrum is unchanged under reflection about integer values of $1/\phi$ and changes sign under translation by one unit in the same quantity. The spectrum is therefore invariant under translation by two units. In the variable κ the equation is invariant under translation with period 2ϕ as anticipated in our analysis of Eq. (1). For rational $\phi=q/p$ the system becomes closed after translation by p periods thus leaving just $2q$ separate equations. Not all these equations are independent, however, as can be seen by making in (4) the substitution

$$C(u)=e^{i(\pi p/2q)u(u-q)}f(u)\,.$$

Indeed, one can then easily verify that $f(u)$ and $f(u+q)$ obey the same equation. If we use Floquet's theorem to connect these two functions through the relation

$$f(u+q)=\exp(2\pi i\mu)f(u)$$

a Hermitian system of q equations for q unknowns results. The secular equation gives then q real solutions for the eigenvalue λ, for each value of the Floquet index μ and of κ. As these indices cover their range, the q roots spread into bands that through (5) give the spectrum for the magnetic field under consideration. As shown in the Appendix the bands thus generated do not overlap and only touching of neighboring bands at their near edges is possible.

Langbein has previously discussed the properties of the secular determinant that results from this treatment.[7] In our notation it has period $2/q$ in κ and the indices μ and κ appear in the constant term only. The equation for λ that results has the form

$$P(\lambda)=(-)^{p+q}[\cos 2\pi p\kappa+2\cos\pi p(\kappa+\tfrac{1}{2}q)\times\cos 2\pi\mu], \tag{7}$$

where $P(\lambda)$ is a polynomial of degree q in λ not containing μ and κ. Inspection of the right-hand side shows that as these indices cover their range it varies between the values -3 and 1.5. Intercepts of the polynomial between these two values define therefore the subbands for the rational field chosen. Figure 1 shows the spectrum obtained in this manner with values of q up to 41. We stopped at this value of q because the symmetries in the spectrum are already visible and bandwidths became as narrow at 10^{-8} in the energy scale of the graph and very time consuming to search for in the computer. The number of subbands equals the denominator of the rational field variable $r=1/\phi$ as expected. Touching of neighboring subbands occurs between the second and third subbands counting from above for the fractional part of $r=\frac{1}{6}$ and its symmetrically equivalent points, and nowhere else in the spectrum. We defer a more detailed study of Fig. 1 until Sec. III. A portion of the energy spectrum as given by (5) is shown in Fig. 2 for $V_1=-U$. The empty lattice Landau levels are included as straight lines. Broadening increases with the field and a fine structure is present between any two integer values of $1/\phi$.

III. PEIERLS SUBSTITUTION METHOD: NESTING

A well-known alternate approach to treating the problem in a Landau basis assumes that the energy function $\epsilon(\vec{k})$ for the lattice with no magnetic field is known. The so called Peierls substitution[10] $\vec{k}\to -i\vec{\nabla}-e\vec{A}/\hbar c$ makes the energy function an operator and the eigenvalue equation to be solved is[13-16]

$$\epsilon(\vec{\nabla}/i-e\vec{A}/\hbar c)\psi=E\psi. \tag{8}$$

As a model for the hexagonal lattice we consider an s tight-binding band with nearest-neighbor

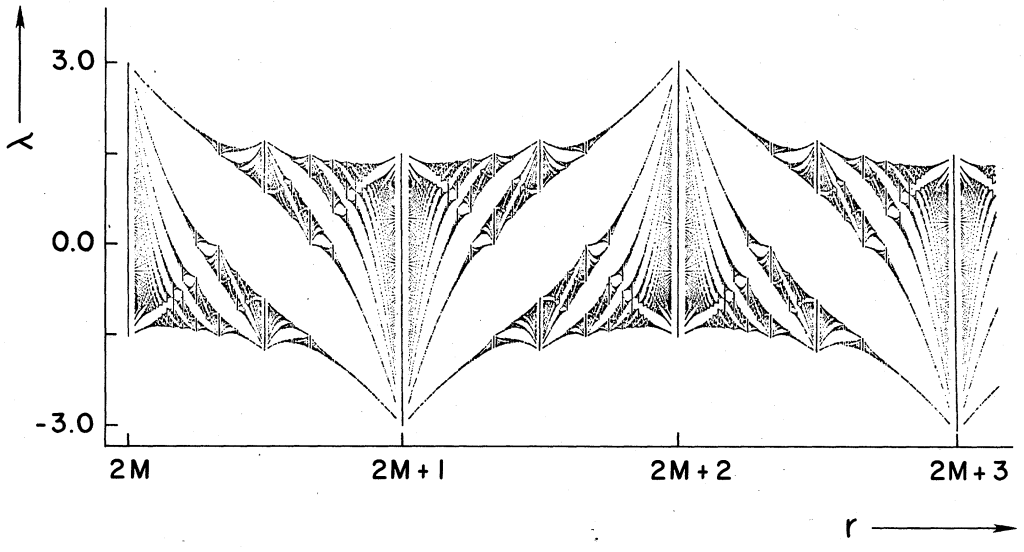

FIG. 1. Spectrum of Eq. (1) for rational values of the variable $1/\phi=r$. M is an arbitrary integer. The spectrum has period 2 in the variable r.

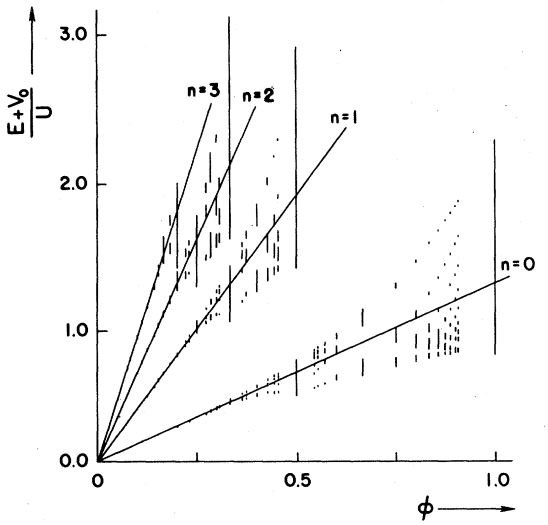

FIG. 2. Energy spectrum for broadened Landau levels with no interlevel mixing. Only low-index levels are shown and the fine structure corresponds to just a few rational values of the field variable ϕ. The empty-lattice Landau levels are represented by slanted straight lines.

overlap only. Using the same orientation of the axes as in Sec. II the energy function that results is

$$\epsilon(\vec{k}) = \epsilon_0 - 2\epsilon_1\{\cos[a(\sqrt{3}k_x - k_y)/2] + \cos ak_y + \cos[a(\sqrt{3}k_x + k_y)/2]\}. \quad (9)$$

In the gauge $\vec{A} = H(0, x, 0)$ the variable y is cyclic and can be separated away from Eq. (8) by the ansatz

$$\psi(x, y) = \exp(i2\pi\nu y/a)b(x)$$

whereupon we obtain using (2), after some algebra, the equation

$$\bar{\lambda}b(\sigma) = \cos\pi\phi(\sigma - \tfrac{1}{2})b(\sigma - 1) + \cos 2\pi\phi\sigma b(\sigma) + \cos\pi\phi(\sigma + \tfrac{1}{2})b(\sigma + 1), \quad (10)$$

where $\sigma = 2x/\sqrt{3}\,a - \nu/\phi$ and $\bar{\lambda}$ is related to the energy through

$$E = \epsilon_0 - 2\bar{\lambda}\epsilon_1. \quad (11)$$

The eigenvalues of (10) then determine the energy spectrum for a given value of the field. Comparing (4) and (10) we see that the present method yields an equation identical in structure to the equation for a single Landau level with the field parameter ϕ replaced by its inverse. This feature is common to the square lattice[17] and was predicted for more general two-dimensional potentials by Langbein.[7] Figure 1 therefore also represents the spectrum of (10) if we interpret the variable r as the field ϕ. A portion of the band-energy spectrum as given by (11) is shown in Fig. 3. Landau levels near the bottom of the field-free band are clearly recognizable, their field dependence in the limit of low field matching exactly the empty-lattice energy levels indicated by straight lines in Fig. 2. Large gaps separate the low-index Landau levels. As the field increases the broadening and structure also matches that in Fig. 2, only the levels bend toward lower energies in Fig. 3. We note that coupling between levels was neglected in Sec. II so that some distortion as the field is increased and the ratio of level to gap width becomes larger, was to be expected. Gaps open up near the top of the band as well thus giving the Landau levels for hole states.

In his detailed numerical study of the square lattice Hofstadter discovered a recursive property which he generalized to all rational values of the field as a nesting hypothesis.[8] We find the spectrum for the hexagonal lattice to have recursive properties as well. A detailed description of nesting may be found in Hofstadter's work and we shall only reformulate it briefly for our case. There are different ways to subdivide the spec-

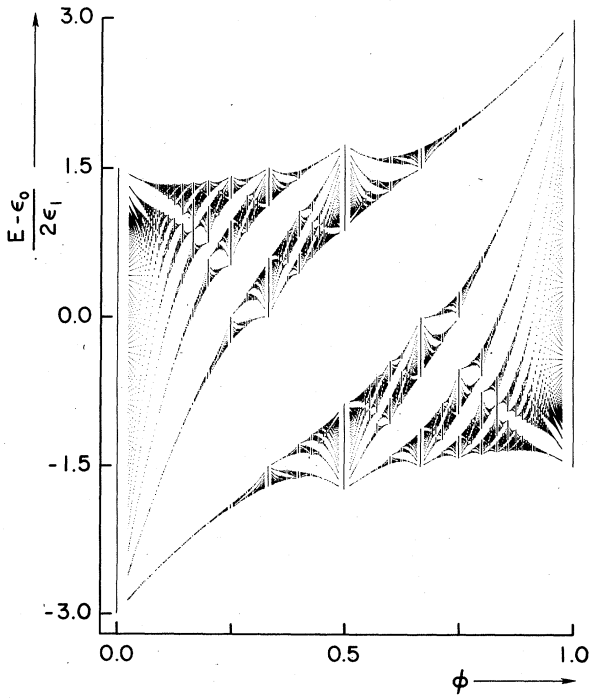

FIG. 3. Energy spectrum for an effective single-band Hamiltonian in the range $0 \leq \phi \leq 1$.

trum to bring about the nesting property. Hofstadter chose as the basic unit the cell $0 \leq \phi < 1$ that covers in his case the fundamental period of the spectrum. We prefer an alternative to Hofstadter's choice and take the entire spectrum as the basic unit with all nested images being replicas of the whole spectrum as well. The advantage is that the fine structure of a single Landau level is then the image of the whole spectrum at the first level of nesting and sub-Landau levels are the image of Landau levels at the next level of nesting, and so on. This subdivision therefore stresses the similarity of Eqs. (4) and (10) as given by the Landau state and band approaches, which appears to be an expression of the nesting property.

In order to formulate the nesting hypothesis we first imagine that a diagonal line has been drawn through the main gap between any two integer values of ϕ. Referring to Fig. 1 this diagonal would rise, for example, from the bottom of the field-free band at $r = 2M + 1$ to the top of the band at $r = 2M + 2$. We next note that these lines separate two basic patterns, one inverted with respect to the other. We proceed to formulate nesting in terms of these patterns in the following way. Call the band at $\phi = 0$ the base line for the whole spectrum that extends from $-\infty$ to ∞. Then, any subband of the spectrum is a base line for a (distorted) direct or inverted copy of the entire spectrum. In going from one level of nesting, say l, to the next level, $l+1$, the local field variables are related through

$$\phi_l - [\phi_l] = \frac{1}{\mathrm{sgn}\{\phi_l - [\phi_l]\} + 1/\phi_{l+1}}, \tag{12}$$

where sgn $\{u\}$ is plus or minus 1 depending on the sign of u, and $[\phi_l]$ denotes the location of the new base line in the old field variable. If this quantity is even, a direct replica of the spectrum is obtained, whereas for $[\phi_l]$ odd the image is inverted. For instance, at the first level of nesting about $[\phi] = 0$ the upper portion that is separated out by the main gap through the cells at either side has the same structure as the entire spectrum, with its local variable ϕ_1 related to ϕ through $\phi = 1/(\mathrm{sgn}\{\phi\} + 1/\phi_1)$. Thus, at $\phi = \pm\frac{1}{2}$ the portion of the spectrum that we are analyzing contains one subband and the local-field value is $\phi_1 = \pm 1$. At $\phi = \pm\frac{2}{3}$ two subbands are found and $\phi_1 = \pm\frac{1}{2}$, etc. The number of subbands strictly follows the rule that it should equal the denominator of the rational fraction in its local-field value. As another example, the center subband at $\phi = \frac{1}{3}$ is characterized by $\phi_2 = -1$ after two steps of successive nesting involving $[\phi] = 0$ and $[\phi_1] = 1$. It belongs to an image of the spectrum anchored about the upper subband at $\phi = \frac{1}{2}$ and bounded by the main gap and the gap going from $\phi = 0$ to the upper edge of the subband at $\phi = \frac{1}{2}$.

The distortion that the spectrum undergoes as it is nested includes a moving over of the touching point between the second and third subbands at $\phi = \frac{1}{6}$. For instance, it appears at $\phi_1 = \frac{1}{5}$ after the first level of nesting about the base line $[\phi] = 0$. Figure 3 shows that this point marks the closing of a gap that originates at the top of the field-free band. In fact, the gap would reappear at larger fields if the sub-Landau levels branching off from the edge of neighboring subbands along the projected path of the gap would trade places. A similar situation occurs below $\phi = \frac{1}{6}$ for gaps that originate at the bottom of the field-free band which would also reappear under a switching of sub-Landau levels. The nesting statement makes no distinction between gaps open or closed in the sense explained above and this adds to the distortion introduced by nesting.

IV. DENSITY OF STATES

The multiplicity of solutions of (7) can be obtained in a straightforward manner since the phases κ and μ appear in the constant term only. We follow the method introduced by Wannier, Obermeir, and Ray that transforms the counting over an energy range to a counting over a range of the polynomial, thus yielding a form of the density of states appropriate for an arbitrary rational value of the field.[17]

Let $\lambda_s(\kappa, \mu)$ be a root of (7) for given κ, μ, and a fixed value of the field. As these indices cover their range the root will scan an entire subband that we have labeled s. The indices have constant weight since they are phase variables and the density of states is then given by the expression

$$g(\lambda) = \left(\frac{1}{q}\right) \sum_{s=1}^{q} \int_0^1 d\kappa \int_0^1 d\mu\, \delta[\lambda_s(\kappa, \mu) - \lambda]. \tag{13}$$

The sum is over all subbands and the total number of states has been normalized to one. The δ function can be integrated over by transforming the integral over μ to an integral over λ_s with the aid of (7), and the remaining integral over κ may be found in tables. One gets

$$g(\lambda) = \left(\frac{1}{2\pi^2}\right) \left|\frac{dP}{d\lambda}\right| \begin{cases} 1/u\,K(v/u), & 1 < P \leq 1.5 \\ 1/v\,K(u/v), & -3 \leq P < 1 \\ 0 & \text{otherwise,} \end{cases} \tag{14}$$

where

$$u = \tfrac{1}{2}\{(P-1)^2 + [(3-2P)^{1/2} + 1]^2\}^{1/2},$$

$$v = (3 - 2P)^{1/4}.$$

P is the value of the polynomial (7) at λ, and $K(x)$ is the complete elliptic integral of the first kind. Within a subband, only this latter factor varies significantly giving a λ-shaped logarithmic singularity to the density of states. At subband edges the density of states drops discontinuously to zero as a gap is encountered.

Although the density of states has the same functional form for all subbands it differs in detail from one subband to another. The total number of states is the same for all subbands however, and it equals $1/q$. To see this we note that $g(\lambda)$ depends on λ through P and its derivative only; the integral over λ is therefore simply transformed to one over P and since the range of the polynomial is the same for all subbands the integral has the same value in all cases. We can use this property to show that below the main gap of Fig. 3 there are exactly ϕ states per unit cell. For this purpose we apply the transformation (12) once about $[\phi]=1$ and obtain for the local variable ϕ_1 that describes the portion of the spectrum below the main gap the relation $\phi_1 = 1 - 1/\phi$. For $\phi = p/q$ this gives $\phi_1 = (p-q)/p$ so that there are p subbands in the region and since each has weight $1/q$ the overall number of states is $p/q = \phi$. Since the degeneracy of Landau levels in the presence of a lattice is just ϕ per unit cell[18] our result gives further evidence that the portion of the spectrum below the main gap indeed corresponds to the lowest Landau level. By repeated application of nesting one can show further that the number of states in the portion enclosed by the main gap and the one directly above it and extending from the bottom of the field-free band to the top of the subband at $\phi = \frac{1}{2}$ is also ϕ, as is for all similar portions further up in the spectrum. This supports then the identification of these portions with Landau levels of higher order.

An interesting alternate description of the spectrum was introduced by one of us (G. H. W.) for the square-lattice case[11] through a plot of the number of states W below each gap versus field. In this plot, the line $W=\phi$ images the main gap of Fig. 3, and the lines $W = 2\phi, 3\phi, \ldots$ image the gaps above it referred to in the preceding paragraph. Similarly, the lines $W = \phi, 2\phi - 1, 3\phi - 2, \ldots$ image the gaps originating at the top and to the left of the band at $\phi = 1$. All gaps in the spectrum and therefore all lines in our plot may be reached by an appropriate nesting of the above structure. One can then show that in the interval $0 \leq \phi < 1$ all gaps are imaged by the set of straight lines $W = M + N\phi$ with M and N integers not both odd and opposite in sign. We note that in the square-lattice case the spectrum has reflection symmetry about a constant-energy line passing through the center of the field-free band, and the integers M and N are unrestricted.[11] For hexagonal lattices this symmetry line does not exist and in fact the gap extending from the top of the band at $\phi = 0$ to the bottom of the band at

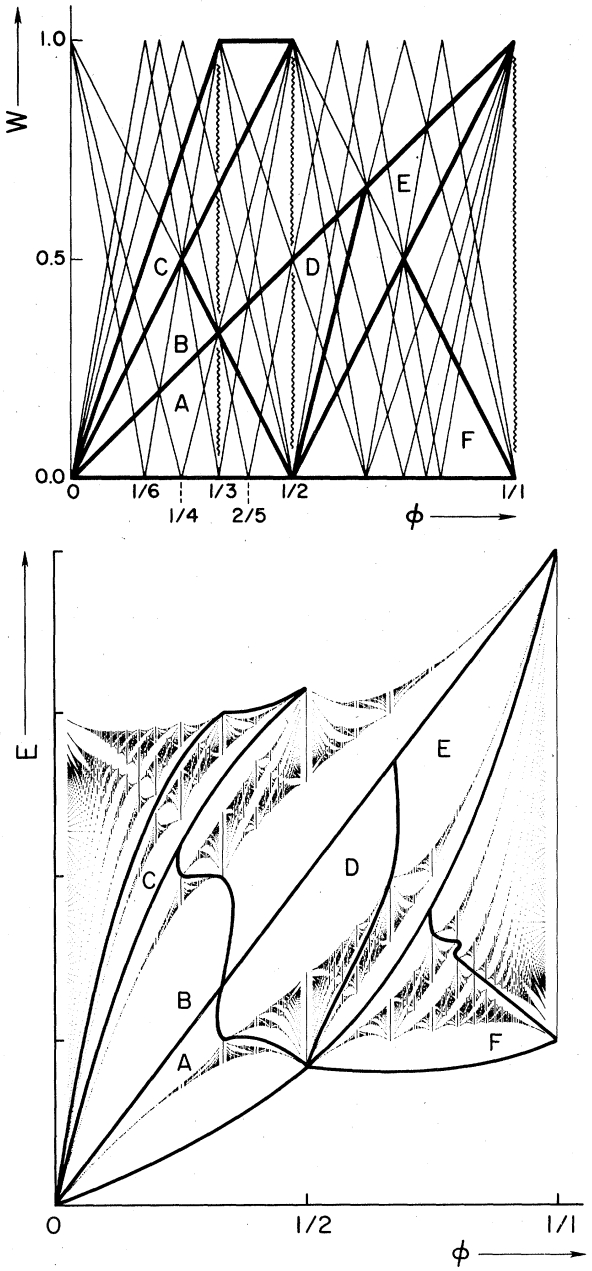

FIG. 4. (a) Statistical weight of states below the main gap in Fig. 3, and its nested replicas. Each line images a gap. Bands in Fig. 3 appear as vertical gaps here, the most prominent of which are shown as wiggly lines. (b) Energy spectrum showing regions bounded by gaps, for comparison with corresponding regions in Fig. 4(a). Note the similarity between regions labeled equally in both figures.

$\phi=1$ is altogether missing, and so are its nested images. This accounts for the restriction imposed on M and N in our case. Figure 4(a) shows a few low-index lines for the hexagonal case. Heavy lines delimit polygons that image regions in the spectrum also shown bounded by heavy lines in Fig. 4(b). We have labeled these regions $A, B, C, \ldots$ for easy identification. Each line in Fig. 4(a) images a gap of Fig. 4(b) and gives the number of states below the gap as a function of the field variable. Conversely, the bands of Fig. 4(b) show as gaps in Fig. 4(a), the most prominent of which at $\phi=1$, $\frac{1}{2}$, and $\frac{1}{3}$ have been fitted in as wiggly lines in Fig. 4(a).

V. CONCLUSIONS

The results presented here for an electron both in the presence of a lattice of hexagonal symmetry and a magnetic field show that the nesting property found previously in the spectrum of the square lattice is of wider validity. In particular, for rational fields the spectrum exhibits a recursive property which can be described by means of a set of simple transformations in the field variable. Furthermore, the correspondence between the alternative treatments that use a Landau basis or the Peierls substitution on an energy-band function is emphasized in our case. This suggests that the equivalence of matrix elements in both methods as found by Langbein[7] and the nesting property are intimately related.

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APPENDIX

In order to prove that no two subbands overlap except possibly at their edge it suffices to show that the polynomial (7) is monotonic everywhere in the allowed band as given by the right-hand side of the expression. In other words, the derivative of the polynomial cannot vanish in that region. If it did vanish for an allowed value of λ then the derivatives of the right-hand side with respect to κ and μ should vanish separately, that is,

$$\sin 2\pi q\kappa + \sin[\pi q(\kappa+\tfrac{1}{2}p)]\cos 2\pi\mu = 0\,, \tag{A1}$$

$$\cos[\pi q(\kappa+\tfrac{1}{2}p)]\sin 2\pi\mu = 0\,. \tag{A2}$$

This is because of the identity

$$\frac{\partial P}{\partial \kappa} = \frac{dP}{d\lambda}\frac{\partial \lambda}{\partial \kappa}$$

and the corresponding one in the variable μ. Note that the above relations are necessary yet not sufficient conditions for the derivative of the polynomial to vanish. If fact, they are always satisfied at band edges as one can show by a procedure similar to that of Ref. 19.

There are three pairs of values of the indices that make the above equations vanish simultaneously, namely, $\mu=\frac{1}{4}(2n+1)$ with $\kappa=-\frac{1}{2}p+(2l+1)/2q$ and $\mu=\frac{1}{2}n$ with either $\kappa=\frac{1}{2}p+(2l+n+1)/q$ or $(2l+n-\frac{1}{2}pq)/3q$. The right-hand side of (7) equals 1 for the first two pairs and, depending on the value of pq, -3.0 or 1.5 for the last pair. The last two values correspond to band edges where (A1) and (A2) are inconclusive, as noted above. The value one is inside the band, however. But just at that point the density of states diverges so there is at least one pair μ, κ that makes $P=1$ yet that does not satisfy (A1) and (A2). This case therefore cannot correspond to a zero of the derivative of the polynomial. We conclude that only at band edges can this occur, thus allowing the touching of neighboring subbands.

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