

Quantum Hall conductances and localization in a magnetic field

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The relation between extended and localized states in a magnetic field is investigated. A general form for the magnetic Bloch states in an arbitrary rational field (with p/q flux quanta through a unit cell, p and q relatively prime integers) is written, and their basic properties are studied. It is shown that the completeness properties of lattices of orbitals relative to a set of N magnetic subbands are connected with the value of the total quantum Hall conductance σ_N (in units of e^2/h) carried by these subbands. In particular, lattices of orbitals can reproduce continuously all the magnetic Bloch states of N subbands if and only if $\sigma_N=0$, a case which may occur only for N multiples of q . This is also the only case where localized magnetic Wannier functions for the subbands can be constructed. In the light of these results a discussion is given of the almost-free-electron limit and the tight-binding approach of Harper's equation.

I. INTRODUCTION

The concepts of Bloch functions¹ and localized orbitals² are basic in the dynamics of electrons in solids. The properties of Bloch functions and localized orbitals, or Wannier functions, have been studied extensively,³⁻⁸ and it is by now well established that these two kinds of quantum states provide equivalent descriptions of bands in solids. Lattices of localized orbitals have also been used to give a global definition and symmetry specification of bands in solids.⁹

In the presence of a uniform magnetic field \mathbf{H} the crystal possesses magnetic translational invariance.¹⁰⁻¹² Because of this symmetry, a band structure exists in the energy spectrum, resulting, in general, from the broadening and splitting of Landau levels in solids.¹³⁻¹⁸ The translational symmetry and band structure in the case $\mathbf{H}\neq\mathbf{0}$ is fundamentally different from that of the classical Bloch case ($\mathbf{H}=\mathbf{0}$). Magnetic translations are essentially translations in a phase space (of the orbit center¹⁹) and not in ordinary space, as in the case of usual translations. Thus, unlike Bloch bands, in which the conserved quantity is the quasimomentum \mathbf{k} , magnetic bands are described by a conserved quantity $\boldsymbol{\kappa}$, which is associated with the whole degree of freedom of the orbit center.¹⁷ While a large amount of information exists concerning Bloch states and localized orbitals for usual bands ($\mathbf{H}=\mathbf{0}$),³⁻⁷ much less is known about the corresponding concepts in the magnetic case, particularly the relation between them.

In a previous paper¹⁷ it was shown that the basic difference between the translational symmetries for $\mathbf{H}=\mathbf{0}$ and $\mathbf{H}\neq\mathbf{0}$ is reflected in a corresponding difference between the Bloch and localized states in the two cases. The case studied was that of a rational magnetic field with $1/N$ flux quanta through a unit cell (N integer). In this case it

was shown that magnetic Bloch states are essentially kq functions²⁰ in the coordinates of the orbit center, and that magnetic lattices (or Pippard networks²¹) of orbitals for a magnetic band are generalized von Neumann lattices.^{22,23} By using known properties of the latter lattices, the completeness properties of Pippard networks of orbitals were investigated. It was shown that exponential localization of magnetic Wannier functions on this network is excluded by their orthogonality. This is in contrast to usual Wannier functions ($\mathbf{H}=\mathbf{0}$), which can be chosen to be exponentially localized.^{3,5,6}

This difference in localization between the Wannier functions for the cases $\mathbf{H}=\mathbf{0}$ and $\mathbf{H}\neq\mathbf{0}$ is due entirely to different periodicities of the corresponding Bloch states in their respective quasimomenta \mathbf{k} and $\boldsymbol{\kappa}$. Bloch functions can always be chosen to be strictly periodic in \mathbf{k} in the Brillouin zone.⁵⁻⁷ As a consequence of this, Wannier functions with exponential localization do exist.^{5,6} On the other hand, the magnetic Bloch states considered in Ref. 17 are kq functions²⁰ in $\boldsymbol{\kappa}$, namely they are periodic in the magnetic Brillouin zone only up to a $\boldsymbol{\kappa}$ -dependent phase factor. Due solely to this fact, magnetic Wannier functions with exponential localization do not exist.¹⁷

In a remarkable paper, Thouless *et al.*²⁴ have shown that the periodicity of the magnetic Bloch states in $\boldsymbol{\kappa}$ has a very interesting physical significance. It determines the quantized Hall conductance $\sigma_j e^2/h$ (σ_j integer) carried by the corresponding magnetic band (or subband) j . In the case of kq periodicity in $\boldsymbol{\kappa}$ (see Ref. 17), $\sigma_j=1$, which corresponds to the Hall conductance e^2/h associated with a Landau level.²⁵ In general, the integer σ_j gives the periodicity conditions in $\boldsymbol{\kappa}$ satisfied by the magnetic Bloch states of an isolated subband j . The integer σ_j satisfies a Diophantine equation,²⁴ which has been shown recently²⁶ to follow just from magnetic translational symmetry. It is

instructive to recall here that an important element in the proof of strict periodicity in \mathbf{k} of the usual Bloch functions ($\mathbf{H}=\mathbf{0}$) is time-reversal symmetry (the Hamiltonian is real).^{6,7} When $\mathbf{H}\neq\mathbf{0}$, the Hamiltonian is not real, so that magnetic Bloch states do not have to be necessarily strictly periodic in \mathbf{k} (in fact, they are not in general). The lack of time-reversal symmetry in the case $\mathbf{H}\neq\mathbf{0}$ is manifested in the fact that a filled magnetic subband carries generally a nonvanishing Hall current ($\sigma_j\neq 0$).²⁴

In a recent paper, Thouless²⁷ shows that Wannier functions for a magnetic subband j can be chosen with exponential localization if and only if $\sigma_j=0$. Thus, a magnetic subband has a representation in terms of exponentially localized magnetic Wannier functions if and only if it does not carry a Hall current. This is a very interesting result. It can, however, be shown that $\sigma_j=0$ for an isolated magnetic band can be achieved only when in the fraction p/q , defining the rationality of the magnetic field, $q=1$. This latter condition can be satisfied only for unphysically high magnetic fields, of the order of 10^9 G. In this paper we show that for N magnetic bands with a total $\sigma_N=0$ (for $N>1$ this can, in principle, be achieved for any magnetic field with the only condition that N is a multiple of q) one can choose N localized orbitals (Wannier functions) that span the N magnetic bands, and reproduce continuously all the magnetic Bloch states. Only in this case localized orbitals and magnetic Bloch states provide equivalent descriptions of magnetic subbands in solids, in analogy with the Bloch case ($\mathbf{H}=\mathbf{0}$).

A description of a set of N subbands by means of symmetry-adapted magnetic Wannier functions was first given by Brown.²⁸ For the case of an arbitrary rational field, with p/q flux quanta through a unit cell (p and q are relatively prime integers), he shows that this description is consistent with the general theory of symmetry-adapted localized orbitals⁴ only if $N=q$, a case which is expected in the framework of the effective Hamiltonian formalism for magnetic fields.²⁹⁻³¹ In a one-band approximation, one finds that the Hamiltonian is represented by the operator $E(\Pi/\hbar)$ (the effective Hamiltonian), where $E(\mathbf{k})$ is the energy function for the given band and Π is the kinetic momentum operator, properly substituted in $E(\mathbf{k})$. An eigenvalue problem for the operator $E(\Pi/\hbar)$, by exploiting its full translational symmetry, gives rise in the tight-binding limit to a one-dimensional difference equation, well known as Harper's,³² or the "almost-Mathieu,"³³ equation. This equation has attracted considerable attention in the recent years, because it emerges naturally in several other problems of solid-state physics where competing periods appear.³⁴ The spectrum of Harper's equation is very sensitive to the exact value of the ratio p/q ,³⁵⁻³⁸ and displays curious recursive³⁸ and scaling³⁹ properties. For a given value of p/q , the spectrum consists of q subbands lying within the range of the function $E(\mathbf{k})$. When equipped with other arguments, this fact leads to the widespread statement that a Bloch band "splits" into q "magnetic subbands" in a rational field p/q . This "splitting" remains, however, controversial.^{17,40}

It is curious that the splitting of a Landau level is also described by Harper's equation, but with p and q inter-

changed (see, e.g., Ref. 24). This expresses a known reciprocity relation between the nearly-free-electron and the tight-binding limits in a magnetic field.⁴¹ Thouless *et al.*²⁴ have calculated from Harper's equation in the two limits the Hall conductances σ_j carried by the magnetic subbands. In the nearly-free-electron limit they have shown for their model that the conductances σ_j of the p split subbands sum to 1 (the conductance of the original Landau level). We show in this paper that this is a general result following from the group-theoretical nature of the splitting of a Landau level. In the tight-binding limit, on the other hand, the conductances σ_j of the q "split" subbands sum to zero.²⁴

In Sec. II of this paper we write a general form for the magnetic Bloch states in an arbitrary rational field p/q , and their basic periodicity properties are considered. One-dimensional Hamiltonians for these states are derived, and the splitting of a Landau level is studied by using the concept of homotopic invariants.⁴² In Sec. III we investigate the completeness properties of magnetic lattices of orbitals relative to a set of N magnetic subbands. It is shown that these properties are intimately connected with the total Hall conductance σ_N carried by the subband. In particular, lattices of orbitals can reproduce continuously all the magnetic Bloch states in the N subbands if and only if $\sigma_N=0$. Only in this case do localized magnetic Wannier functions for the subbands exist. These results are applied to the nearly-free-electron limit and to the effective Hamiltonian approach of Harper's equation.

II. BLOCH STATES IN A RATIONAL MAGNETIC FIELD

In this section the general form of the Bloch states in an arbitrary rational magnetic field is written, and their basic properties are studied. The Hamiltonian of an electron (of charge $-e$ and mass m) moving in a periodic potential $V(\mathbf{r})$ and a uniform magnetic field \mathbf{H} is

$$\mathcal{H} = \frac{\Pi^2}{2m} + V(\mathbf{r}), \quad (1)$$

where Π is the kinetic momentum,

$$\Pi = \mathbf{p} + \frac{e}{2c} \mathbf{H} \times \mathbf{r} \equiv \mathbf{p} + \frac{1}{2} \boldsymbol{\beta} \times \mathbf{r}, \quad \boldsymbol{\beta} = e\mathbf{H}/c \quad (2)$$

expressed in the symmetric gauge. For the sake of clarity we shall restrict ourselves in this paper to the relevant case of motion in a two-dimensional crystal perpendicular to \mathbf{H} . The crystal lattice is assumed to be rectangular with basis vectors \mathbf{a}_1 and \mathbf{a}_2 directed along the x and y axes, respectively, of a coordinate system (x, y) . The extension to more general lattice geometry (including the third dimension) can be carried out without much difficulty.^{16,43} The magnetic field \mathbf{H} satisfies the general rationality condition

$$\frac{\mathbf{H} \cdot \mathbf{a}_1 \times \mathbf{a}_2}{hc/e} = \frac{p}{q}, \quad (3)$$

where p and q are relatively prime integers. Condition (3) implies a commensurability between the crystal lattice and the magnetic lattice whose unit cell encloses one quantum

of flux, hc/e . Namely, a superlattice with basis vectors $\mathbf{b}_1 = q_1 \mathbf{a}_1$ and $\mathbf{b}_2 = q_2 \mathbf{a}_2$ (q_1 and q_2 are integers satisfying $q_1 q_2 = q$) can be found, such that its unit cell (built on \mathbf{b}_1 and \mathbf{b}_2) encloses precisely p flux quanta. On this superlattice one can define an Abelian group of magnetic translations^{11,12} commuting with the Hamiltonian (1):

$$(-1)^{n_1 n_2 p} T(\mathbf{b}_n) = (-1)^{n_1 n_2 p} \exp \left[\frac{i}{\hbar} \Pi_c \cdot \mathbf{b}_n \right], \quad (4)$$

where $\mathbf{b}_n \equiv n_1 \mathbf{b}_1 + n_2 \mathbf{b}_2$ (n_1 and n_2 are all integers) and

$$\Pi_c = \mathbf{p} - \frac{1}{2} \boldsymbol{\beta} \times \mathbf{r}. \quad (5)$$

The operator (5) gives the center of the classical orbit in a magnetic field, $(x_0, y_0) = (-\Pi_{cy}/\beta, \Pi_{cx}/\beta)$.⁴⁴ The components of the operators (2) and (5) can be associated with pairs of canonical variables (\bar{Q}, \bar{P}) and (Q, P) , given by^{17,19}

$$\bar{Q} = \frac{1}{\beta} \Pi_y, \quad \bar{P} = \Pi_x, \quad [\bar{Q}, \bar{P}] = i\hbar, \quad (6)$$

$$Q = y_0 = \frac{1}{\beta} \Pi_{cx}, \quad P = -\beta x_0 = \Pi_{cy}, \quad [Q, P] = i\hbar.$$

The variables (6) define two phase planes (\bar{Q}, \bar{P}) and (Q, P) for the kinetic momentum and the center of the magnetic orbit, respectively. Here, as in Ref. 17, we shall work in the \bar{P} representation. In the absence of the periodic potential, the Hamiltonian (1) reads

$$\mathcal{H}_0 = \frac{\Pi^2}{2m} = \frac{\bar{P}^2}{2m} + \frac{m\omega^2 \bar{Q}^2}{2}, \quad \omega = \frac{eH}{mc}; \quad (7)$$

namely, it is a harmonic oscillator in the (\bar{Q}, \bar{P}) phase plane with eigenenergies (Landau levels)

$$E_l = \hbar\omega(l + \frac{1}{2}). \quad (8)$$

Because of the absence of the (Q, P) canonical pair in (7), there is much arbitrariness in the choice of the eigenfunctions of (7), which is directly related to the infinite degeneracy of the Landau levels (8).¹⁷ This choice is fixed by requiring simultaneous eigenfunctions of (7) and of a complete set of commuting operators in the (Q, P) phase plane. An important case of such a complete set of operators is the Abelian group of magnetic translations

$$(-1)^{n_1 n_2} T(\mathbf{b}'_n) = (-1)^{n_1 n_2} \exp \left[\frac{i}{\hbar} \Pi_c \cdot \mathbf{b}'_n \right], \quad (9)$$

where $\mathbf{b}'_n \equiv n_1 \mathbf{b}'_1 + n_2 \mathbf{b}'_2$, and the unit cell built on \mathbf{b}'_1 and \mathbf{b}'_2 encloses exactly one quantum of flux, hc/e . The simultaneous eigenfunctions of (7) and (9) are

$$\psi_{l\kappa}^{(0)}(\bar{P}, P) = f_l(\bar{P}) \langle P | \kappa \rangle, \quad (10)$$

where $f_l(\bar{P})$ is an oscillator function in \bar{P} , corresponding to the levels (8), and

$$\langle P | \kappa \rangle = \left[\frac{\hbar b'_1}{2\pi} \right]^{1/2} \sum_{n=-\infty}^{\infty} \exp(-i\kappa_1 n b'_1) \times \delta \left[P - \hbar\kappa_2 - \frac{2\pi\hbar}{b'_2} n \right] \quad (11)$$

is a q distribution²⁰ in the variable P , with $\kappa \equiv (\kappa_1, \kappa_2)$ (the magnetic quasimomentum) specifying the eigenvalues $\exp(i\kappa \cdot \mathbf{b}'_n)$ of (9). Since the group (9) is a complete set of operators in the (Q, P) phase plane, its eigenfunctions (11) form a complete set of functions in the variable P , when κ ranges in the magnetic Brillouin zone

$$0 \leq \kappa_1 \leq 2\pi/b'_1, \quad 0 \leq \kappa_2 \leq 2\pi/b'_2. \quad (12)$$

Correspondingly, the set of functions (10), at fixed l , spans the space of a Landau level, and thus describes completely its infinite degeneracy.¹⁷

In the presence of the periodic potential, the Hamiltonian (1) commutes with the Abelian group (4). Because of this magnetic translational symmetry, a band structure is expected in the energy spectrum of (1). The eigenfunctions (magnetic Bloch states) $\psi_{j\kappa}(\bar{P}, P)$ of (1) are labeled by a magnetic band index j and a magnetic quasimomentum κ specifying the eigenvalues of (4). The group (4) is actually a subgroup of index p of the group (9),¹² since, by definition of (4) and (9), we can choose, for example, $\mathbf{b}'_1 = \mathbf{b}_1/p$, $\mathbf{b}'_2 = \mathbf{b}_2$ (this choice will be made from now on, together with $\mathbf{b}_1 = q\mathbf{a}_1$, $\mathbf{b}_2 = \mathbf{a}_2$). Thus all the p distributions

$$\langle P | \kappa_1 + 2\pi s/a_1, \kappa_2 \rangle, \quad s = 0, 1, \dots, p-1,$$

in (11) are eigenfunctions of (4) with the same eigenvalues $\exp(i\kappa \cdot \mathbf{b}_n)$. It follows that the most general form of $\psi_{j\kappa}(\bar{P}, P)$ is

$$\psi_{j\kappa}(\bar{P}, P) = \sum_{s=0}^{p-1} \phi_{j\kappa}^{(s)}(\bar{P}) \langle P | \kappa_1 + 2\pi s/a_1, \kappa_2 \rangle, \quad (13)$$

where κ now ranges in the zone

$$0 \leq \kappa_1 \leq \frac{2\pi}{b_1}, \quad 0 \leq \kappa_2 \leq 2\pi/b_2, \quad (14)$$

which is p times smaller than the zone (12). For an isolated magnetic band j , the functions (13) must satisfy periodicity conditions in κ in the zone (14). Following arguments similar to those given in Ref. 45, the phase of $\psi_{j\kappa}(\bar{P}, P)$ can always be chosen so that these conditions read as follows:

$$\psi_{j\kappa_1 + 2\pi/b_1, \kappa_2}(\bar{P}, P) = \psi_{j\kappa}(\bar{P}, P), \quad (15a)$$

$$\psi_{j\kappa_1, \kappa_2 + 2\pi/b_2}(\bar{P}, P) = \exp(i\sigma_j \kappa_1 b_1) \psi_{j\kappa}(\bar{P}, P), \quad (15b)$$

where σ_j is an integer generally dependent on the band j . As was shown in Ref. 24, and as it will be discussed in more detail below, σ_j gives the Hall conductance of the magnetic band j . Given the conditions (15), we may easily derive from them and from (13) corresponding conditions for the p functions $\phi_{j\kappa}^{(s)}(\bar{P})$ in (13):

$$\phi_{j\kappa_1 + 2\pi/b_1, \kappa_2}^{(s)}(\bar{P}) = \phi_{j\kappa}^{(s+t)}(\bar{P}), \quad (16a)$$

where $t \equiv 1 \pmod{q}$, $s+t$ defined mod p , and

$$\phi_{j\kappa_1, \kappa_2 + 2\pi/b_2}^{(s)}(\bar{P}) = \exp \left[-i \frac{q}{p} 2\pi s + i\sigma_j q \kappa_1 a_1 - i \frac{q}{p} \kappa_1 a_1 \right] \times \phi_{j\kappa}^{(s)}(\bar{P}). \quad (16b)$$

Equations for the functions $\phi_{j\kappa}^{(s)}(\bar{P})$ can be obtained by substituting (13) into the Schrödinger equation with the Hamiltonian (1). Expanding the periodic potential in a Fourier series,

$$\sum_{s'=0}^{p-1} \sum_{u,n=-\infty}^{\infty} v_{up+|s-s'|_p,n} \exp \left[\frac{i}{\hbar} \frac{q}{p} \left(\hbar\kappa_1 + \frac{2\pi\hbar s}{a_1} - \bar{P} \right) na_1 \right] \times \exp \left[\frac{i}{\hbar} \frac{q}{p} (\beta\bar{Q} - \hbar\kappa_2)(up + |s-s'|_p a_2) \right] \phi_{j\kappa}^{(s')}(\bar{P}) = [E_j(\kappa) - \mathcal{H}_0] \phi_{j\kappa}^{(s)}(\bar{P}), \quad (18)$$

where $|s-s'|_p \equiv s-s' \pmod{p}$, $E_j(\kappa)$ is the magnetic energy band, and \mathcal{H}_0 is the Landau Hamiltonian. Equations (18), for $s=0,1,\dots,p-1$, form a system of p coupled differential equations for the p functions $\phi_{j\kappa}^{(s)}(\bar{P})$. This system of equations has for each κ an infinite number of solutions with the index j running from 1 to ∞ . The system of equations (18) is apparently periodic in κ_2 with the period $2\pi p/qa_2$. However, it is not hard to see that the period in κ_2 is actually smaller than this. In fact, introducing the functions

$$\bar{\phi}_{j\kappa}^{(s)}(\bar{P}) = \exp \left[i\kappa_2 \frac{q}{p} sa_2 \right] \phi_{j\kappa}^{(s)}(\bar{P}), \quad (19)$$

it is easily verified that (19) satisfies a system of equations periodic in κ_2 with the period $2\pi/(qa_2)$. This period is q times smaller than that figuring in condition (16b), and it can be shown to be related with the well-known q -fold degeneracy in a magnetic band.¹¹⁻¹³ After the transformation (19), the system (18) becomes periodic in κ_1 and κ_2 in the zone

$$0 \leq \kappa_1 \leq 2\pi p/qa_1, \quad 0 \leq \kappa_2 \leq 2\pi/qa_2. \quad (20)$$

Given a definite solution $\phi_{j\kappa}^{(s)}(\bar{P})$, $s=0,1,\dots,p-1$, of (18), corresponding to an isolated magnetic band j , the functions (19) must satisfy periodicity conditions in κ in the zone (20). Again following arguments similar to those given in Ref. 45, the phase of $\bar{\phi}_{j\kappa}^{(s)}(\bar{P})$ can be chosen so to make $\bar{\phi}_{j\kappa}^{(s)}(\bar{P})$ strictly periodic in κ_1 with the period $2\pi p/qa_1$ [this is consistent with (16a)], while

$$\bar{\phi}_{j\kappa_1, \kappa_2+2\pi/qa_2}^{(s)}(\bar{P}) = \exp \left[-im_j \kappa_1 \frac{qa_1}{p} \right] \bar{\phi}_{j\kappa}^{(s)}(\bar{P}), \quad (21)$$

where m_j is an integer generally dependent on j . Using (19), we see that relation (21) is consistent with condition (16b) if and only if

$$p\sigma_j + qm_j = 1. \quad (22)$$

Equation (22) is an important Diophantine equation for the integers σ_j and m_j . It was derived recently on the basis of symmetry arguments.²⁶ In fact, it follows from the q -fold degeneracy in a magnetic band, mentioned above. The integer σ_j has the meaning of the Hall conductance (in units of e^2/h) carried by the magnetic band j .²⁴

The spectrum of the Hamiltonian (1) can be calculated

$$V(x,y) = \sum_{m,n} v_{m,n} \exp \left[2\pi i \left(\frac{mx}{a_1} + \frac{ny}{a_2} \right) \right], \quad (17)$$

and using (2), (5), (6), and (13), we obtain, after some algebraic manipulations,

perturbatively in the limit of a weak periodic potential in the framework of a single Landau level.^{14,24,41} This approach has a sound group-theoretical basis.^{12,13} In fact, the space, or the infinite degeneracy of a Landau level, is described by the complete group of operators (9).^{17,19} In the presence of a periodic potential the Hamiltonian commutes with the group (4), which describes the space of an isolated magnetic band. Since the group (4) is a subgroup of index p of the group (9),¹² it follows that a Landau level should split, in group-theoretical terms, into p magnetic bands (hereafter called subbands). We shall number the subbands split from a Landau level l by the index w , $w=1,2,\dots,p$. Thus, in this framework we may write $j \equiv (l,w)$, and the functions $\phi_{j\kappa}^{(s)}(\bar{P})$ read simply as follows:

$$\phi_{j\kappa}^{(s)}(\bar{P}) = f_l(\bar{P}) c_{lw}^{(s)}(\kappa), \quad (23)$$

where $c_{lw}^{(s)}(\kappa)$ are functions of κ to be determined from the corresponding Eq. (18). A detailed discussion of these equations is given in Ref. 43 with the result that they lead to a splitting of the Landau level into p subbands. This splitting is accompanied by an interesting sum rule which we prove below. The total Hall conductance carried by the p split subbands is equal to that of the original Landau level, namely 1 (in units of e^2/h):

$$\sum_{w=1}^p \sigma_{lw} = 1. \quad (24)$$

To prove relation (24), we notice first that after the transformation (19), one obtains from Eq. (18) a $p \times p$ matrix $W_{ss'}^{(l)}(\kappa)$ ($s,s'=0,1,\dots,p-1$) with eigenvectors $c_{lw}^{(s)}(\kappa)$ ($w=1,2,\dots,p$). This matrix describes the splitting of the Landau level l into p subbands and is periodic in κ in the zone (20). It is known⁴² that if the eigenvalues $E_{lw}(\kappa)$ of such a matrix are distinct at each κ (the magnetic subbands are isolated), one can associate with each subband $E_{lw}(\kappa)$ a homotopic invariant equal to the integer m_{lw} appearing in the periodicity conditions (21). For a finite $p \times p$ matrix the set of p integers m_{lw} ($w=1,2,\dots,p$) must satisfy the sum rule⁴²

$$\sum_{w=1}^p m_{lw} = 0. \quad (25)$$

Using relation (25) in Eq. (22), the sum rule (24) follows. It is interesting to notice that from Eq. (22) it follows also that, for $p > 1$, no one of the integers m_{lw} in relation (25)

can vanish. This means that for $p > 1$ the system of equations (18) admits no solution strictly periodic in κ in the zone (20). Similarly, for $q > 1$, $\sigma_{lw} \neq 0$ in relation (24), so that the magnetic Bloch states (13) are never strictly periodic in κ in the zone (14). This remark will be referred to later in discussing the localization problem.

An important well-studied case²⁴ arises in the nearly-free-electron limit with the simple periodic potential

$$V(x,y) = 2V_1 \cos \left[\frac{2\pi x}{a_1} \right] + 2V_2 \cos \left[\frac{2\pi y}{a_2} \right]. \quad (26)$$

The difference equation for the potential (26) is known as Harper's³² or the "almost-Mathieu"³³ equation, and has been studied extensively in recent years,³⁵⁻³⁹ also in connection with several other problems in solid-state physics.³⁴ Thouless *et al.*²⁴ have calculated the Hall conductances σ_w associated with the magnetic subbands $E_w(\kappa)$ for the potential (26). Analogous calculations were performed in the case of a hexagonal lattice.⁴⁶

By using the magnetic Bloch functions (13), one can develop the quantum-mechanical representation which generalizes the magnetic Adams representation developed in Ref. 17 for the special case $p = 1$. We begin by writing the orthogonality relations satisfied by the eigenfunctions (13). For each κ the system of equations (18) correspond to a Hermitian problem, so that using (11) and (15) we obtain

$$\int \int d\bar{P} dP \psi_{j\kappa}^*(\bar{P}, P) \psi_{j\kappa'}(\bar{P}, P) = \delta_{jj'} \hat{\Delta}_j(\kappa - \kappa'),$$

$$\hat{\Delta}_j(\kappa - \kappa') \equiv \sum_{n_1, n_2} \delta \left[\kappa_1 - \kappa'_1 - \frac{2\pi n_1}{b_1} \right] \exp(-i\sigma_j \kappa_1 b_1 n_2)$$

$$\times \delta \left[\kappa_2 - \kappa'_2 - \frac{2\pi n_2}{b_2} \right]. \quad (27)$$

We have also the completeness relation

$$\sum_j \int d\kappa \psi_{j\kappa}^*(\bar{P}, P) \psi_{j\kappa}(\bar{P}', P') = \delta(\bar{P} - \bar{P}') \delta(P - P'), \quad (28)$$

where the integral over κ is performed in the zone (14). By using the formalism of Ref. 17 and the relations (27) and (28), we obtain the periodicity conditions obeyed by a wave function $B_j(\kappa)$ in the Adams representation [see relations (15)]:

$$B_j(\kappa_1 + 2\pi/b_1, \kappa_2) = B_j(\kappa_1, \kappa_2), \quad (29a)$$

$$B_j(\kappa_1, \kappa_2 + 2\pi/b_2) = \exp(-i\sigma_j \kappa_1 b_1) B_j(\kappa_1, \kappa_2). \quad (29b)$$

Expressions for operators in the Adams representation are obtained in complete analogy with the special case $p = 1$ (see Ref. 17).

The main feature of the magnetic Adams representation is its characterization by an entire series of integers σ_j , $j = 1, 2, 3, \dots$, as we see, for example, from (27) and (29). The set $\{\sigma_j\}$ is not completely arbitrary. Thus, if two subbands, say j_1 and j_2 , first overlap ("collide") and then separate again, one has the sum rule⁴²

$$\sigma_{j_1} + \sigma_{j_2} = \sigma'_{j_1} + \sigma'_{j_2}, \quad (30)$$

where the prime indicates the case after the collision. The sum rule (30) (and similar expressions for the simultaneous collision of three or more subbands) represents physically the conservation law of the total Hall conductance of the colliding subbands. If collisions take place only within a Landau level, the sum rule (24) is maintained for each l . More generally, the integer σ_j of a subband may change only after a collision with another subband takes place, but then the sum rule (30) must be satisfied. These facts put restrictions on the set of integers $\{\sigma_j\}$.

In the limit of a weak periodic potential, the magnetic Bloch states assume the following important form, obtained by substituting (23) into (13):

$$\psi_{j\kappa}(\bar{P}, P) = f_l(\bar{P}) g_{lw\kappa}(P), \quad (31)$$

where

$$g_{lw\kappa}(P) = \sum_{s=0}^{p-1} c_{lw}^{(s)}(\kappa) \langle P | \kappa_1 + 2\pi s/a_1, \kappa_2 \rangle. \quad (32)$$

In relation (31) one has an explicit separation of variables \bar{P} and P . The index w in (31) and (32) is a good quantum number, having a sound group-theoretical origin and labeling the p subbands into which a single Landau level splits. The corresponding p eigenvectors $c_{lw}^{(s)}(\kappa)$ ($w = 1, 2, \dots, p$) are orthogonal and linearly independent at each κ . The functions (31), for $w = 1, 2, \dots, p$ and κ ranging in the zone (14), thus span the space of a Landau level, and are therefore completely equivalent to the set of functions (10), where κ ranges in the zone (12) [which is p times larger than (14)]. This equivalency reflects the group-theoretical splitting of a Landau level into p magnetic subbands.¹²⁻¹⁴

III. MAGNETIC LATTICES OF ORBITALS

In this section we investigate completeness properties of lattices of orbitals for magnetic subbands in solids. These properties were studied in our previous work¹⁷ for the special case $p = 1$, with $\sigma_j = 1$ for all j . It was shown there that a lattice of orbitals generated by the complete group of magnetic translations (9) is essentially a von Neumann lattice^{22,23} in the (Q, P) phase plane, spanning the Hilbert space of a magnetic band. It was also shown that orthogonal orbitals on this lattice, namely magnetic Wannier functions, are necessarily poorly localized at least in one direction of space (have power-law localization in this direction). Recently Thouless²⁷ has shown that a magnetic subband j can have a representation in terms of exponentially localized magnetic Wannier functions if and only if $\sigma_j = 0$. This is a very interesting result and it can be generalized to a number of magnetic bands with the total $\sigma = 0$. Actually, the result for a number of magnetic bands is of much physical interest for the following reason. From relation (22) it follows that only when $q = 1$ can σ be zero for a particular magnetic band. The value $q = 1$ corresponds, however, to nonphysical magnetic fields (of the order of 10^9 G). On the other hand, when one considers q magnetic bands, then relation (22) for the total σ of these q bands is

$$p\sigma + qm = q \quad (33)$$

Unlike relation (22), which has a solution $\sigma=0$ only for $q=1$, relation (33) for the q bands has always a solution $\sigma=0$. Having this in mind, we develop in what follows a set of localized orbitals for q magnetic bands.

A magnetic lattice or Pippard network²¹ of orbitals for a subband j' is obtained by applying the group of magnetic translations (4) to a general orbital $A_{j'}(\bar{P}, P)$ belonging to this subband. This orbital is

$$A_{j'}(\bar{P}, P) = \int d\kappa B_{j'}(\kappa) \psi_{j'\kappa}(\bar{P}, P), \quad (34)$$

where $B_{j'}(\kappa)$ is a general function of κ satisfying the periodicity conditions (29). In the Adams representation the orbital (34) reads $\delta_{j,j'} B_{j'}(\kappa)$. By operating with the magnetic translations (4), we obtain the magnetic lattice of orbitals

$$(-1)^{n_1 n_2 p} T(\mathbf{b}_n) \delta_{j,j'} B_{j'}(\kappa) = \delta_{j,j'} \exp(i\kappa \cdot \mathbf{b}_n) B_{j'}(\kappa). \quad (35)$$

Consider the Hilbert space of all square-integrable functions $\delta_{j,j'} G(\kappa)$ belonging to subband j' . The set of functions (35) for all \mathbf{b}_n is complete in this Hilbert space, provided the function $B_{j'}(\kappa)$ does not vanish in a finite area of the zone (14) (this latter requirement is always satisfied by physical, localized orbitals). The proof of this completeness is just the same as that given in Ref. 17 in the special case $p=1$.

An important property of a function $B_{j'}(\kappa)$ satisfying the periodicity conditions (29) is the following: If $B_{j'}(\kappa)$ is continuous in the variable κ , it must assume at least $|\sigma_{j'}|$ zeros in the zone (14), where each zero is counted a number of times equal to its multiplicity. For $\sigma_{j'}=1$, this is the known theorem of zeros of kq functions.²² The proof of the theorem for general values of $\sigma_{j'}$ is given in the Appendix. The requirement of continuity of $B_{j'}(\kappa)$ is physically a requirement of localization of the corresponding orbital (34). In fact, a necessary condition for the exponential localization of (34) in both the x and y directions is the analyticity of $B_{j'}(\kappa)$ in the κ_1 and κ_2 complex planes.^{43,17} As was already noticed previously,^{17,27} this exponential localization is not possessed by a lattice of magnetic Wannier functions in the case $\sigma_{j'} \neq 0$. It is instructive to show this again by using the theorem above. From the requirement of orthogonality of (35) at different sites \mathbf{b}_n , one obtains (compare with Ref. 17)

$$B_{j'}(\kappa) = C \exp[i\tau(\kappa)], \quad (36)$$

where C is some constant, and the phase $\tau(\kappa)$ is a real function of κ . Since the function (36) can never vanish, it must be discontinuous for $\sigma_{j'} \neq 0$. The corresponding magnetic Wannier functions cannot have, therefore, exponential localization in both the x and y directions. This localization can be achieved only in the case²⁷ $\sigma_{j'}=0$, where one can choose, for example, $B_{j'}(\kappa)=1$ in (36). However, because of Eq. (22), the value $\sigma_{j'}=0$ may arise (and in fact, it arises in specific models^{24,46}) only when $q=1$, a case corresponding to physically unaccessible fields $H \sim 10^9$ G [see (3)]. According to Thouless,²⁷ the positions of the discontinuities of $B_{j'}(\kappa)$ for $\sigma_{j'} \neq 0$ may be interpreted as the locations where the $|\sigma_{j'}|$ units of Hall

current, carried by subband j' , are "concentrated" in the representation of the magnetic lattice of orbitals (35).

Assuming the continuity of $B_{j'}(\kappa)$, one can derive another completeness property of the set of functions (35): The magnetic lattice of orbitals (35) is overcomplete in the Hilbert space of subband j' by at least $|\sigma_{j'}|$ members, namely it remains complete if $|\sigma_{j'}|$ orbitals are removed, but it may become incomplete if another orbital is removed. This result is a simple consequence of the theorem above and the known relation between zeros and overcompleteness derived in connection with von Neumann lattices.²³

Having considered the completeness properties of the magnetic lattice of orbitals (35) relative to the Hilbert space of a subband, we now examine these properties in the corresponding space of the extended magnetic Bloch states (13). To derive these states from the orbital (34), one should apply to it the projection operator of the magnetic translation group (4).¹⁰ This is equivalent to forming the following linear combination of the orbitals (35) [which we now express in the (\bar{P}, P) representation]

$$\begin{aligned} \bar{\psi}_{j'\kappa}(\bar{P}, P) &\equiv \frac{p\hbar}{2\pi\beta} \sum_n \exp(-i\kappa' \cdot \mathbf{b}_n) (-1)^{n_1 n_2 p} \\ &\quad \times T(\mathbf{b}_n) A_{j'}(\bar{P}, P) \\ &= B_{j'}(\kappa') \psi_{j'\kappa}(\bar{P}, P). \end{aligned} \quad (37)$$

For $\sigma_{j'} \neq 0$ the function $B_{j'}(\kappa')$ either vanishes or is discontinuous at some points $\kappa' = \kappa_0$. At these points the magnetic Bloch states $\psi_{j'\kappa}(\bar{P}, P)$ cannot be expressed by definite linear combinations of the orbitals (35). In other words, for $\sigma_{j'} \neq 0$ the space of all magnetic Bloch states of subband j' cannot be reproduced continuously by the magnetic lattice of orbitals (35). This should be compared with the Bloch case ($\mathbf{H}=\mathbf{0}$), where it is known⁴⁻⁸ that the Bloch states $\psi_{m\mathbf{k}}(\mathbf{r})$ of band m can always be expressed as linear combinations of a lattice of orbitals $\varphi_m(\mathbf{r}-\mathbf{t}_n)$ (\mathbf{t}_n are the crystal lattice sites):

$$\psi_{m\mathbf{k}}(\mathbf{r}) = \frac{1}{(V_b)^{1/2}} B^{-1}(\mathbf{k}) \sum_n \exp(-i\mathbf{k} \cdot \mathbf{t}_n) \varphi_m(\mathbf{r}-\mathbf{t}_n), \quad (38)$$

where V_b is the volume of a Brillouin zone, and $B(\mathbf{k})$ is the function defined by

$$\varphi_m(\mathbf{r}) = \frac{1}{(V_b)^{1/2}} \int d\mathbf{k} B(\mathbf{k}) \psi_{m\mathbf{k}}(\mathbf{r}). \quad (39)$$

For the linear combination in (38) to be definite at all \mathbf{k} , the function $B(\mathbf{k})$ must be chosen continuous and non-vanishing. This is possible because of the fact that Bloch states can be chosen to be strictly periodic in \mathbf{k} in the Brillouin zone.³⁻⁷ For example, one may choose simply $B(\mathbf{k})=1$, which corresponds to Wannier functions² in (39). In the magnetic case strict periodicity in κ in the basic zone (14) ($\sigma_{j'}=0$) can be achieved only for nonphysical fields corresponding to $q=1$ (for this value of q the two lattices \mathbf{b}_n and \mathbf{t}_n coincide). Thus, in all physical cases, the descriptions of a magnetic subband by a lattice

of orbitals and by the set of all its magnetic Bloch states are not equivalent.

We shall now generalize the ideas above to a set of N subbands. Obviously, in order to span the Hilbert spaces of these subbands, one needs N magnetic lattices of orbitals (35), one for each subband. However, the basic idea here is to consider the set of N subbands as one single entity. This entity will be described by N independent magnetic lattices built on N different orbitals $A_s(\bar{P}, P)$, $s = 1, 2, \dots, N$, each belonging, in general, to all N subbands, say $j = 1, 2, \dots, N$:

$$A_s(\bar{P}, P) = \sum_{j=1}^N \int d\kappa B_j^{(s)}(\kappa) \psi_{j\kappa}(\bar{P}, P). \quad (40)$$

By applying to (40) the group of magnetic translations (4), one obtains the N lattices of orbitals (expressed in the Adams representation)

$$(-1)^{n_1 n_2 p} T(\mathbf{b}_n) B_j^{(s)}(\kappa) = \exp(i\kappa \cdot \mathbf{b}_n) B_j^{(s)}(\kappa), \quad s, j = 1, 2, \dots, N. \quad (41)$$

Consider the Hilbert space of all square-integrable functions $G_j(\kappa)$ belonging to the N subbands. The set of orbitals (41) is complete in this Hilbert space if, from the requirement of orthogonality of $G_j(\kappa)$ with all the members of this set, it follows that $G_j(\kappa)$ corresponds to the zero state. The requirement above gives the $N \times N$ system of equations

$$\sum_{j=1}^N G_j^*(\kappa) B_j^{(s)}(\kappa) = 0, \quad (42)$$

$s = 1, 2, \dots, N$. Consider the determinant $\Delta_N(\kappa)$ of the $N \times N$ matrix built on the functions $B_j^{(s)}(\kappa)$. For general physical orbitals in (40), $\Delta_N(\kappa)$ does not vanish in a finite area of the zone (14). Then from (42) it follows that for almost all κ , $G_j(\kappa) = 0$, which proves the completeness of the set (41).

We now consider the possibility of reproducing continuously all the magnetic Bloch states in the N subbands from the N lattices of orbitals (41). By applying to each orbital (40) the projection operator of the magnetic translation group (4), one obtains, in analogy to (37), a set of N functions $\bar{\psi}_{s\kappa}(\bar{P}, P)$, $s = 1, 2, \dots, N$:

$$\bar{\psi}_{s\kappa}(\bar{P}, P) = \sum_{j=1}^N B_j^{(s)}(\kappa) \psi_{j\kappa}(\bar{P}, P). \quad (43)$$

The functions (43) are labeled by the "magnetic band index" s , and are strictly periodic in κ in the zone (14) [namely, they satisfy conditions (15) with $\sigma_s = 0$ for each s]. The orbitals (40) can be rewritten as follows:

$$A_s(\bar{P}, P) = \int d\kappa \bar{\psi}_{s\kappa}(\bar{P}, P). \quad (44)$$

By associating each orbital (40) with a "magnetic band" s , the form (44) becomes quite analogous to that of usual Wannier functions² in the case $H = 0$. In order to reproduce continuously all the original magnetic Bloch states $\psi_{j\kappa}(\bar{P}, P)$, $j = 1, 2, \dots, N$, from the set of functions (43), the $N \times N$ matrix $B_j^{(s)}(\kappa)$ in (43) must be continuous and invertible at each κ . Only in this case are the new magnetic bands s equivalent to the original ones j . We now

show that the two requirements above on $B_j^{(s)}(\kappa)$ are compatible if and only if the total Hall conductance σ_N carried by the N subbands $j, j = 1, 2, \dots, N$, vanishes:

$$\sigma_N \equiv \sum_{j=1}^N \sigma_j = 0. \quad (45)$$

Physically, condition (45) is an expression of the conservation law (30) in going from a set of subbands s with a total $\sigma = 0$ (since $\sigma_s = 0$ for all s) to a set of subbands j with $\sigma_N = 0$. To show this we notice first that the determinant $\Delta_N(\kappa)$ of the matrix $B_j^{(s)}(\kappa)$ satisfies the periodicity conditions (29) with σ_N replacing σ_j . Then, if $\Delta_N(\kappa)$ is continuous, it must vanish at some κ for $\sigma_N \neq 0$, and the matrix $B_j^{(s)}(\kappa)$ is not invertible there. When $\sigma_N = 0$, the matrix $B_j^{(s)}(\kappa)$ can always be chosen to be nonsingular, in fact, unitary. This is accomplished by choosing $B_j^{(s)}(\kappa)$, $s = 1, 2, \dots, N$, to be the N orthonormal eigenvectors of a periodic Hermitian matrix $A(\kappa)$ whose homotopic invariants are precisely σ_j , and $\sigma_N = 0$. Such a matrix can always be constructed explicitly.⁴² This completes the proof of our claim.

By choosing the matrix $B_j^{(s)}(\kappa)$ to be unitary in the case $\sigma_N = 0$, the functions (43) become orthonormal magnetic Bloch states for the N subbands s , which are equivalent to the subbands j . It is also easy to show that with this choice of $B_j^{(s)}(\kappa)$ the N lattices of orbitals (41) become a localized orthonormal set (magnetic Wannier functions). Condition (45) is compatible with relation (22) only if N is a multiple of q . Thus, in conclusion, the magnetic Bloch states in N subbands can be reproduced continuously from the N lattices of orbitals (41) if and only if $\sigma_N = 0$. Only in this case it is possible to construct localized magnetic Wannier functions reproducing continuously a set of q (or a multiple of q) subbands. This construction generalizes that given in Ref. 27 for a single subband to q subbands. For a single subband j the condition $\sigma_j = 0$ is satisfied, because of relation (22), only for $q = 1$, which corresponds to unrealistic magnetic fields. On the other hand, the construction of localized magnetic Wannier functions for q subbands, with a total $\sigma = 0$, should be applicable to physically achievable fields.

In what follows we shall consider two important instances where sets of subbands are described by magnetic lattices of orbitals. The first case is the limit of a weak periodic potential. Here a Landau level splits into p subbands, and the magnetic Bloch states are given by (31) and (32). It is known that the infinite degeneracy of a Landau level is completely accounted for by the so-called Pippard network of localized orbitals,^{21,19} which is obtained by applying to an arbitrary orbital $f_l(\bar{P})g(P)$ belonging to the Landau level [$g(P)$ is a general square-integrable function of P] the Abelian group of magnetic translations (9):^{19,17}

$$(-1)^{n_1 n_2} T(\mathbf{b}'_n) f_l(\bar{P}) g(P). \quad (46)$$

The set of orbitals (46) is a special case of (35) for $p = 1$, and spans the Hilbert space of a Landau level. By choosing $\mathbf{b}'_1 = \mathbf{b}_1/p$, $\mathbf{b}'_2 = \mathbf{b}_2$, and using the fact that (4) is a subgroup of (9), the set (46) can be rewritten as follows:

$$(-1)^{n_1 n_2 p} T(\mathbf{b}_n) f_l(\bar{P}) g_s(P). \quad (47)$$

Here we have introduced the p functions $g_s(P)$, $s=0,1,\dots,p-1$,

$$g_s(P) \equiv T \left[\frac{s \mathbf{b}_1}{p} \right] g(P) = \sum_{w=1}^p \int d\kappa B_w^{(s)}(\kappa) g_{w\kappa}(P), \quad (48)$$

and we have expanded $g_s(P)$ in the complete set of functions (32). By writing (46) in the form (47) with (48), it becomes evident that the p magnetic lattices (47), spanning the Hilbert space of the p split subbands $w=1,2,\dots,p$, actually span at the same time the Hilbert space of the original Landau level. The two Hilbert spaces are identical because of the group-theoretical nature of the splitting. It should be noticed, however, that, since the total Hall conductance carried by the p subbands does not vanish [see relation (24)], the magnetic Bloch states (31) cannot be reproduced continuously from p magnetic lattices (47).

The second case we consider is the tight-binding limit of a Bloch electron in a magnetic field. Here one looks for an approximate eigenfunction of the Hamiltonian in the form of a linear combination of orbitals, properly displaced on the crystal lattice by magnetic translations:

$$\psi^{(m)}(\mathbf{r}) = \sum_n c(\mathbf{t}_n) T(\mathbf{t}_n) \varphi_m(\mathbf{r}), \quad (49)$$

where \mathbf{t}_n is the crystal lattice, the operator $T(\mathbf{t}_n)$ is defined as in (4), and $\varphi_m(\mathbf{r})$ is an atomic orbital for band m . The form (49) was originally proposed by Peierls,²⁹ who used it in order to show that the coefficients of expansion $c(\mathbf{t}_n)$ in (49) are eigenfunctions of the effective Hamiltonian $E_m(\Pi/\hbar)$ obtained by properly substituting the kinetic momentum operator (2) in the expression $E_m(\mathbf{k})$ for the energy band. The eigenvalues of $E_m(\Pi/\hbar)$ should correspond to the energy eigenvalues within the tight-binding band m . The original and usual approach to the effective Hamiltonian makes use of the WKB approximation, leading to the semiclassical quantization of the energy contours $E_m(\mathbf{k}) = \text{const}$ in reciprocal space.⁴⁷⁻⁴⁹ In later work³⁵⁻³⁸ the full translational symmetry of the operator $E_m(\Pi/\hbar)$ was taken into account. A well-studied case is that corresponding to the tight-binding band³²

$$E_m(\mathbf{k}) = 2E_0 [\cos(k_x a_1) + \cos(k_y a_2)], \quad (50)$$

where a_1 and a_2 are the lattice constants. After the substitution $\mathbf{k} \rightarrow \Pi/\hbar$, where Π is given by (2), one obtains a differential operator $E_m(\Pi/\hbar)$ in the xy representation. Its eigenfunctions are $c(\mathbf{r})$, where $c(\mathbf{t}_n)$ should be identified with the expansion coefficients in (49). Writing

$$c(\mathbf{r}) = \exp \left[-i\mu x - i\nu y + \frac{i\beta xy}{2\hbar} \right] g(x/a_1), \quad (51)$$

where $g(x/a_1)$ satisfies the periodicity condition

$$g(x/a_1 + q) = g(x/a_1), \quad (52)$$

one obtains from the effective Hamiltonian the following eigenvalue problem for $g(s)$ [s is now a dimensionless discrete variable ranging, because of (52), in the interval $0 \leq s \leq q-1$]:

$$E_0 \left[\exp(-i\mu a_1) g(s+1) + \exp(i\mu a_1) g(s-1) + 2 \cos \left[\frac{2\pi p}{q} s - \nu a_2 \right] g(s) \right] = E g(s). \quad (53)$$

The one-dimensional difference equation (53) was derived originally by Harper,³² and its properties were investigated extensively in the last several years,^{33,35-39} also in connection with other problems in solid-state physics,³⁴ where this equation emerges. Because of condition (52), one obtains from (53) a system of q linear equations. For each "quasimomentum" (μ, ν) , the corresponding eigenvalue problem admits q eigenvalues, which form q bands $E_j(\mu, \nu)$, $j=1,2,\dots,q$, $0 \leq \mu < 2\pi/a_1$, $0 \leq \nu < 2\pi/a_2$.

Let us consider the periodicity properties of Eq. (53) in the "quasimomentum" (μ, ν) . Equation (53) is periodic in both μ and ν with the periods $2\pi/a_1$ and $2\pi/a_2$. However, as in the case of Eq. (18), it is not hard to see that the period in μ is actually smaller than $2\pi/a_1$. In fact, introducing the functions

$$\bar{g}_{j\mu\nu}(s) = \exp(-i\mu s a_1) g_{j\mu\nu}(s), \quad j=1,2,\dots,q \quad (54)$$

where s is taken mod q , the system of equations for (54) is periodic in μ with the period $2\pi/qa_1$. Equation (53) thus corresponds to the eigenvalue problem of a $q \times q$ matrix which is periodic in μ and ν with exactly the same periods defining the basic zone (14). As previously mentioned in connection with the eigenvalue problem for weak periodic potentials, the eigenvectors (54) of such a matrix can be assigned integers \tilde{m}_j , $j=1,2,\dots,q$,⁴² determining the periodicity conditions in (μ, ν) satisfied by them [compare with Eq. (21)]:

$$\bar{g}_{j\mu+2\pi/qa_1, \nu}(s) = \bar{g}_{j\mu\nu}(s), \quad (55a)$$

$$\bar{g}_{j\mu, \nu+2\pi/a_2}(s) = \exp(i\tilde{m}_j \mu q a_1) \bar{g}_{j\mu\nu}(s). \quad (55b)$$

The integers \tilde{m}_j must satisfy a sum rule analogous to (25):⁴²

$$\sum_{j=1}^q \tilde{m}_j = 0. \quad (56)$$

We can substitute (51) with $\mathbf{r} = \mathbf{t}_n = n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2$ into expression (49) and use (54) to obtain functions $\psi_{j\mu\nu}^{(m)}$ having magnetic translational symmetry. Let us assume that these functions correspond to actual magnetic Bloch states for q subbands in a solid, with (μ, ν) playing the role of the magnetic quasimomentum κ . Then, by using (55) in (49), it is easily verified that the functions $\psi_{j\kappa}^{(m)}$ satisfy the periodicity conditions (15) with $\sigma_j = \tilde{m}_j$. Because of relation (56), the total Hall conductance carried by the q subbands is thus $\sigma_q = 0$. We can therefore use the transformations (43) and (44) for defining q localized orbitals A_s , $s=1,2,\dots,q$, that reproduce continuously the q subbands. However, this is precisely what one assumes when writing the basic relation (49), which underlines the effective Hamiltonian approach.⁵⁰ We thus see that Harper's equation forms a consistent framework for describing q magnetic subbands carrying a total Hall conductance $\sigma_q = 0$.

However, the basic assumption above, that the solutions

of Harper's equation and the associated eigenfunctions $\psi_{j\mu\nu}^{(m)}$ give the actual energy spectrum for the problem, should be carefully examined. It is known^{35,38} that the spectrum of Harper's equation is quite sensitive to the values of the integers p and q , whose ratio p/q defines the magnetic field [see relation (3)], but separately have no physical meaning. The average energy gap in the spectrum is proportional to $1/q$, so that slight variations in the magnetic field cause drastic changes in the energy spectrum. The spectrum is also periodic in p/q with period 1 (corresponding to one flux quantum, or a very high field of the order of 10^9 G), and is symmetric relative to $p/q = 1/2$, so that the energy spectra for low fields ($p/q, q \gg p$) are identical to those for high fields ($p'/q' = 1 - p/q$).³⁸ These properties of Harper's equation are physically strange and doubtful, especially in view of the fact that the effective Hamiltonian $E_m(\Pi/h)$ is known to have corrections in the form of an asymptotic expansion in powers of the magnetic field.³¹ These corrections may well be of the order of the energy gaps for $q \gg 1$, and may therefore affect significantly the general structure (in particular, the periodicity and symmetry properties) of the spectrum as predicted from Harper's equation. We would also like to point out that not in all cases can a set of q subbands with $\sigma_q = 0$ be found. In fact, for $p = 1$, and at least in the limit of a weak periodic potential, each magnetic band (broadened Landau level) carries a Hall conductance $\sigma_j = 1$,¹⁷ so that $\sigma_q = q$ and can never vanish. For $p > 1$, and in the same limit, model calculations^{24,46} show that sets of q subbands with $\sigma_q = 0$ do exist, and the Hall conductances σ_j can be calculated from Eq. (18). Taking a number of Landau levels, say s , they will split into sp magnetic subbands. Among them it may be possible to find q subbands with $\sigma_q = 0$, and it is then possible to construct, by means of the transformations (43) and (44), localized magnetic Wannier functions spanning these subbands. This is just an example of our general result that q magnetic subbands with $\sigma_q = 0$ can be described by a set of localized orbitals.

IV. SUMMARY

In this paper the basic properties of magnetic Bloch states and localized orbitals in an arbitrary rational magnetic field have been studied. Because of the lack of time-reversal symmetry in the problem, magnetic Bloch states, unlike usual Bloch states,⁴⁻⁷ do not have to be strictly periodic in the quasimomentum κ . For an isolated magnetic subband, they satisfy the general periodicity conditions (15), where σ_j is an integer giving the Hall conductance carried by the subband.²⁴ Because of magnetic translational symmetry,²⁶ σ_j has to satisfy the Diophantine equation (22). Moreover, the group-theoretical nature of the splitting of a Landau level imposes the sum rule (24) on the Hall conductances carried by the p split subbands.

A set of N magnetic subbands can be described by N lattices of orbitals. The completeness properties of these orbitals relative to the set of subbands are found to be intimately connected with the total Hall conductance σ_N carried by the subbands. In particular, only for $\sigma_N = 0$ (a case which may occur only for N multiples of q) can lat-

tices of localized orbitals reproduce continuously all the magnetic Bloch states in N subbands. In this case it is possible to construct q lattices of localized magnetic Wannier functions spanning q subbands with $\sigma_q = 0$. These results have been used to analyze the nearly-free-electron limit and the effective Hamiltonian approach of Harper's equation. It has been shown that Harper's equation forms a consistent framework for describing q magnetic subbands with $\sigma_q = 0$. However, because of asymptotic corrections to the effective Hamiltonian,³¹ the fine structure of the energy spectrum, as predicted from Harper's equation,^{35,38} may not be relevant physically.

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APPENDIX

We show here that a continuous function of κ , $B_j(\kappa)$, satisfying the periodicity conditions (29), must assume at least $|\sigma_j|$ zeros in the basic zone (14), where each zero is counted a number of times equal to its multiplicity (the theorem of zeros). To show this, let us assume the contrary, namely that $B_j(\kappa)$ assumes zeros at the f points κ_s , $s = 1, 2, \dots, f$, with respective multiplicities n_s such that

$$n_T \equiv \sum_{s=1}^f n_s < |\sigma_j|. \quad (\text{A1})$$

Consider the function

$$A(\kappa) = \exp \left[-\frac{\hbar p}{2\beta} \kappa^2 \right] \theta_3(z|\tau), \quad (\text{A2})$$

where $z = b_1(\kappa_1 + i\kappa_2)/2$, $\tau = ib_1/b_2$, and $\theta_3(z|\tau)$ is a theta function.⁵¹ The function (A2) is continuous (actually entire) in κ , satisfies conditions (29) with $\sigma_j = 1$, and assumes precisely one simple zero in the zone (14) at $\kappa = (\pi/b_1, \pi/b_2)$.⁵¹ The position of this zero can be displaced everywhere in the zone (14) by operating on (A2) with an arbitrary magnetic (phase-plane) translation $T(t)$. Let $A_s(\kappa)$ denote the function (A2), but with its simple zero located at $\kappa = \kappa_s$. We form the product

$$A_T(\kappa) \equiv \prod_{s=1}^f [A_s(\kappa)]^{n_s}. \quad (\text{A3})$$

The function (A3) satisfies conditions (29) with $\sigma_j = n_T$ and assumes the same zeros and respective multiplicities as the function $B_j(\kappa)$. Therefore, the function

$$B_j(\kappa)/A_T(\kappa) \quad (\text{A4})$$

is well defined, continuous, and does not vanish. However, the function (A4) satisfies conditions (29) with [recall (A1)] $\sigma_j = \sigma_j - n_T \neq 0$. Following the same arguments as in the theorem of zeros of kq functions,^{22,23} one can prove that such a function must assume at least one zero, thus leading to a contradiction.

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