

## Quantized Hall effect in a hexagonal periodic potential

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(Received 31 October 1983)

The Hall conductivity of a two-dimensional electron gas in a strong magnetic field and a hexagonal periodic potential is discussed. The hexagonal potential is treated by separating it into a term which depends on only one coordinate and a second term, treated perturbatively, which depends on both coordinates. Emphasis is placed on the origin of the differences between the hexagonal potential case and the square-lattice potential case discussed earlier by Thouless *et al.* [Phys. Rev. Lett. **49**, 405 (1982)]. The calculations are based on a simple physical criterion for determining the Hall conductivity which has been justified starting from the Kubo formula.

### I. INTRODUCTION

Much recent interest in the Hall conductance of a two-dimensional electron gas  $\sigma_H$  has been sparked by the experimental observation that it can be quantized in units of  $e^2/h$ .<sup>1</sup> It is now generally believed that this quantization must occur whenever the Fermi level  $\epsilon_F$  lies in a gap between bulk states of the system or in a region of localized electronic states (e.g., Refs. 2–6). The case of electrons in a high magnetic field and a weak periodic potential is particularly interesting because of its unusual electronic structure.<sup>7–9</sup> In this case each Landau level is split into  $p$  nonoverlapping subbands where  $p/q$  is the number of flux quanta piercing one unit cell of the periodic potential, i.e.,

$$\frac{HA_0}{\Phi_0} = \frac{p}{q}, \quad (1)$$

where  $A_0$  is the unit cell area and  $\Phi_0 = hc/e$  is the flux quantum.<sup>10</sup> When the Fermi level lies in the gap between  $t$ th and  $(t+1)$ st subband, the Hall conductivity

$$\sigma_H = \frac{e^2 \sigma_t}{h}, \quad (2)$$

where  $\sigma_t$  is an integer. Thouless *et al.*<sup>11</sup> have given an expression for  $\sigma_t$  for the case of a square-lattice potential. More recently, Yoshioka<sup>12</sup> has determined  $\sigma_t$  numerically for several values of  $p/q$  for a hexagonal periodic potential. In this article we expand on the analytic treatment given by Thouless *et al.*, and generalize it to the case of a hexagonal potential. Emphasis is placed on explaining the physical origin of the substantial differences which exist between the two cases.

In the next section we rederive the expression for the Hall conductivity in terms of the wave-vector dependence of the eigenfunctions originally proposed in Ref. 11. From this formula, we derive a criterion for determining  $\sigma_H$ , which is made the basis of subsequent work. In Sec. III we consider a potential with one term, proportional to the parameter  $V_1$ , dependent on only one coordinate and a second term, proportional to the parameter  $V_2$ , dependent

on both coordinates. This potential is such that it equals the hexagonal lattice potential when  $V_2 = V_1$ , but, following Thouless *et al.*,<sup>11</sup> we begin by considering the case  $|V_2| \ll |V_1|$ . Unlike the case of the square-lattice potential, in the hexagonal case the Hall conductivities in some gaps change as a function of  $|V_2|/|V_1|$ . These changes in  $\sigma_t$  are always associated with the closing of a gap between subbands (band crossings). In Sec. IV we show that most of these band crossings can be understood by means of simple arguments. In so doing we provide a partial explanation for the absence of any such crossings in the square-lattice case. Finally in Sec. V we summarize our findings and present some concluding remarks.

### II. HALL CONDUCTIVITY AND WAVE-VECTOR DEPENDENCE OF THE EIGENFUNCTIONS

Our aim in this section is to justify a simple criterion for selecting a value of  $\sigma_t$  which will be made the basis of subsequent work. For a finite system with quasi-periodic-boundary conditions the most fundamental available starting point is the Kubo formula. For noninteracting electrons with the Fermi energy in a gap, this may be expressed quite generally in the form

$$\sigma_H = \frac{2e^2 \hbar}{L^2} \sum_{\alpha, \beta} \frac{\Theta_\alpha^\leftarrow \Theta_\beta^\rightarrow}{(\epsilon_\alpha - \epsilon_\beta)^2} \text{Im}(\langle \alpha | V_x | \beta \rangle \langle \beta | V_y | \alpha \rangle), \quad (3)$$

where  $V_x$  and  $V_y$  are the components of the velocity operator,  $\{\epsilon_\alpha, |\alpha\rangle\}$  denotes the eigenvalues and eigenfunctions of the Hamiltonian, and  $L^2$  is the area within which the periodic boundary conditions are applied. In Eq. (3),

$$\Theta_\alpha^\leftarrow \equiv \Theta(\epsilon_F - \epsilon_\alpha), \quad \Theta_\alpha^\rightarrow \equiv \Theta(\epsilon_\alpha - \epsilon_F).$$

If we choose a Landau gauge so that the vector potential  $\vec{A}$  is given by

$$\vec{A} = (0, Hx - \delta A, 0), \quad (4)$$

where  $\delta A$  is arbitrary, the eigenstates of the Hamiltonian in the absence of the periodic potential are given by

$$\langle \vec{r} | k_y, n \rangle = \frac{1}{\sqrt{L_y}} \exp(ik_y y) \phi_n(x - a_L^2 k_y - \delta A/H), \quad (5a)$$

$$E_{k_y, n} = \hbar \omega_c (n + \frac{1}{2}), \quad (5b)$$

where  $\omega_c = eH/mc$ ,  $a_L^2 = \Phi_0/2\pi H$ , and  $\phi_n(x)$  is the  $n$ th eigenfunction of the one-dimensional harmonic oscillator. It is sometimes more useful to label these states by the  $x$  coordinates about which they are centered,  $X \equiv a_L^2 k_y + \delta A/H$ . The allowed values of  $X$  are fixed by requiring  $k_y L$  to be a multiple of  $2\pi$ . For a general two-dimensional periodic potential it is always possible to choose the coordinate axes so that one of the primitive reciprocal-lattice vectors lies along the  $x$  axis, i.e.,

$$\vec{G}_1 = (Q_0, 0), \quad (6a)$$

$$\vec{G}_2 = (Q_1, Q_2). \quad (6b)$$

Then the potential can be expanded,

$$V(x, y) = \sum_{n, m} V_{n, m} \exp[i(nQ_0 + mQ_1)x + mQ_2 y]. \quad (7)$$

If we now restrict our attention to the lowest Landau level ( $n=0$ ) and take  $\hbar\omega_c/2$  as the zero of energy, then the matrix elements of the Hamiltonian are

$$\begin{aligned} \langle X' | H | X \rangle &= \sum_{n, m} V_{n, m} \exp\left\{-\frac{1}{4}[(nQ_0 + mQ_1)^2 + m^2 Q_2^2] a_L^2\right\} \\ &\quad \times \exp\left[\frac{1}{2}i(nQ_0 + mQ_1)(X + X')\right] \\ &\quad \times \delta(X' - X - ma_L^2 Q_2). \end{aligned} \quad (8)$$

Noting that  $a_L^2 Q_2 Q_0/2\pi = \Phi_0/HA_0 = q/p$ , restricting  $k_y$  to the interval  $[0, Q_2]$ , assuming that  $Q_1/Q_0 = s/t$ , and defining

$$X_{i, l}(k_y) \equiv a_L^2 k_y + i \left[ \frac{2\pi q}{Q_0 p} \right] + l \left[ \frac{2\pi j q}{Q_0 p} \right] + \frac{\delta A}{H}, \quad (9)$$

$i = 1, \dots, j,$

it follows that  $\langle X_{n', l'}(k'_y) | H | X_{n, l}(k_y) \rangle$  is zero unless  $k_y = k'_y$ , and that this matrix element is unchanged when  $l$  and  $l'$  are simultaneously shifted. [In Eq. (9),  $j$  equals  $pt$  divided by the largest common factor of  $t$  and  $q$ .] This periodicity motivates the introduction of another wave vector, making the unitary transformation to a basis set

$$|k_x, k_y; i\rangle = \frac{1}{\sqrt{S}} \sum_l \exp[ik_x X_{i, l}(k_y)] |X_{i, l}(k_y)\rangle, \quad (10)$$

where  $S = LQ_0 p / (2\pi j q)$  and  $k_x \in [0, Q_0 p / j q]$ . Then both  $k_x$  and  $k_y$  are good quantum numbers, and all eigenfunctions and eigenvalues required for evaluating the Kubo formula [Eq. (3)] may be determined by diagonalizing a small matrix.<sup>13</sup>

In discussing  $\sigma_H$ , it is more convenient to deal with the auxiliary functions  $u_\alpha(\vec{k})$ , related to the eigenfunction  $\psi_\alpha(\vec{k})$  by

$$u_\alpha(\vec{k}) = \exp(-i\vec{k} \cdot \vec{r}) \psi_\alpha(\vec{k}). \quad (11)$$

These functions obey  $\vec{k}$ -independent boundary conditions [ $u_\alpha(x, y + 2\pi/Q_2) = u_\alpha(x, y)$  and  $u_\alpha(x + 2\pi j q / Q_0 p, y) = \exp(ij Q_2 y) u_\alpha(x, y)$ ] and are eigenfunctions of a  $\vec{k}$ -dependent effective Hamiltonian,

$$H_{\text{eff}}(\vec{k}) = \frac{1}{2m} \left[ \left[ -i\hbar \frac{\partial}{\partial x} + \hbar k_x \right]^2 + \left[ -i\hbar \frac{\partial}{\partial y} + \hbar k_y - \frac{eHx}{c} \right]^2 \right] + V(x, y). \quad (12)$$

(We have set  $\delta A$  to zero.) In terms of the  $u$  eigenfunctions,<sup>14</sup>

$$\begin{aligned} \sigma_H &= \frac{e^2}{\pi \hbar} \int_{\text{BZ}} d\vec{k} \sum_{\alpha, \beta} \frac{\Theta_\alpha^<(\vec{k}) \Theta_\beta^>(\vec{k})}{[\epsilon_\alpha(\vec{k}) - \epsilon_\beta(\vec{k})]^2} \\ &\quad \times \text{Im} \left\langle u_\alpha(\vec{k}) \left| \frac{\partial H_{\text{eff}}}{\partial k_x} \right| u_\beta(\vec{k}) \right\rangle \\ &\quad \times \left\langle u_\beta(\vec{k}) \left| \frac{\partial H_{\text{eff}}}{\partial k_y} \right| u_\alpha(\vec{k}) \right\rangle. \end{aligned} \quad (13)$$

To proceed further, we follow Ref. 11 in replacing the derivatives on the Hamiltonian by derivatives on the eigenfunctions. Since the eigenvalue equation determines these functions only to within a position-independent phase factor there is a great deal of freedom in choosing them. For the moment, we require only that they be analytic functions of  $\vec{k}$ . Then, noting that

$$\begin{aligned} \left\langle u_\alpha(\vec{k}) \left| \frac{\partial H_{\text{eff}}}{\partial \vec{k}} \right| u_\beta(\vec{k}) \right\rangle &= [\epsilon_\alpha(\vec{k}) - \epsilon_\beta(\vec{k})] \\ &\quad \times \left\langle \frac{\partial u_\alpha(\vec{k})}{\partial \vec{k}} \left| u_\beta(\vec{k}) \right\rangle, \quad \alpha \neq \beta \end{aligned} \quad (14)$$

we have

$$\sigma_H = \frac{e^2}{\pi \hbar} \int_{\text{BZ}} d\vec{k} \sum_\alpha \Theta_\alpha^<(\vec{k}) \text{Im} \left\langle \frac{\partial u_\alpha(\vec{k})}{\partial k_x} \left| \frac{\partial u_\alpha(\vec{k})}{\partial k_y} \right\rangle \quad (15)$$

$$= \frac{e^2}{2\pi \hbar} \oint_{\text{BZ}} \sum_\alpha \Theta_\alpha^< \text{Im} \left\langle u_\alpha(\vec{k}) \left| \frac{\partial u_\alpha(\vec{k})}{\partial k} \right\rangle \cdot d\vec{k}, \quad (16)$$

where the last integral is around the perimeter of our rectangular Brillouin zone. We can always choose one component of  $|\partial u_\alpha(\vec{k})/\partial \vec{k}\rangle$ , for example,  $|\partial u_\alpha(\vec{k})/\partial k_y\rangle$ , to be orthogonal to  $|u_\alpha(\vec{k})\rangle$ . With this choice it follows that

$$\sigma_H = \frac{e^2}{2\pi \hbar} \sum_\alpha \Theta_\alpha^< \int_0^{Q_0 p / j q} dk_x \frac{d\Theta_\alpha(k_x)}{dk_x}, \quad (17)$$

where  $u_\alpha(k_x, k_y = Q_2) = \exp[-i\Theta_\alpha(k_x)] u_\alpha(k_x, k_y = 0)$ . Thus in the intra-Landau-level gaps,  $\sigma_H$  is an integral

multiple of  $e^2/h$ . In what follows, we discuss how that integer is determined.

We define

$$\exp(-i\vec{k}\cdot\vec{r})\langle\vec{r}|k_x, k_y; i\rangle \equiv \langle\vec{r}|u_i(\vec{k})\rangle.$$

If all terms in the potential [Eq. (7)] with  $m \neq 0$  are set to zero and we stay within the Hilbert space of the lowest Landau level,  $|u_i(\vec{k})\rangle$  is an eigenfunction of  $H_{\text{eff}}(\vec{k})$ . At some values of  $k_y$ , the eigenvalues will cross, but as the  $m \neq 0$  terms in the potential are turned on, anticrossings centered about these  $k_y$  values occur and open up the intra-Landau-level gaps. For simplicity we shall assume in this paragraph that  $j=p$ , so that at a given  $k_y$  and a given energy only one crossing occurs.<sup>15</sup> We consider the evolution of the wave function as a function of  $k_y$  near  $k_y^*$  the value where bands  $i$  and  $i'$  cross when the  $m \neq 0$  terms in the potential are turned off. For the sake of definiteness we assume that  $i' > i$ , and define

$$\langle X_{i',l}(k_y) | H | X_{i,l}(k_y) \rangle \equiv V_-(k_y), \quad (18a)$$

$$\langle X_{i',l-1}(k_y) | H | X_{i,l}(k_y) \rangle \equiv V_+(k_y). \quad (18b)$$

As discussed in more detail in Sec. IV, other indirect couplings between  $i$  and  $i'$  can be treated as effective contributions to  $V_+(k_y)$  and  $V_-(k_y)$ . Near  $k_y^*$  we need only consider the  $2 \times 2$  Hamiltonian matrix

$$\underline{H}(\vec{k}) = \begin{bmatrix} \epsilon_i(k_y) & V \\ V^* & \epsilon_{i'}(k_y) \end{bmatrix}, \quad (19)$$

where  $X_+ = X_{i,l+1} - X_{i',l}$ ,  $X_- = X_{i,l} - X_{i',l}$ , and  $V$  is defined below. The two eigenstates may be chosen to be

$$|u_{\pm}(\vec{k})\rangle = c_i^{\pm}(\vec{k}) |u_i(\vec{k})\rangle + c_{i'}^{\pm}(\vec{k}) |u_{i'}(\vec{k})\rangle, \quad (20a)$$

$$\begin{aligned} \phi &= -\arg(V(k_y^{(2)})) + \int_{k_y^{(1)}}^{k_y^{(2)}} |c_i^-(\vec{k})|^2 \frac{d}{dk_y} \arg(V) + a_L^2 k_x (k_y^{(2)} - k_y^{(1)}) \\ &= a_L^2 k_x (k_y^{(2)} - k_y^{(1)}) - \int_{k_y^{(1)}}^{k_y^{(2)}} dk_y \arg(V) \frac{d}{dk_y} |c_i^-(\vec{k})|^2. \end{aligned} \quad (23)$$

The first term in Eq. (23), when substituted into Eq. (17), yields the contribution to the classical Hall current, which is  $e^2/hp$  for each of the  $p$  subbands of the Landau level. The second term in Eq. (23) gives, as a contribution to  $\sigma_H$ ,

$$\begin{aligned} &\frac{e^2}{2\pi h} \int_0^{Q_0/q} dk_x \arg(V(k_y^*)) \\ &= \frac{e^2}{h} \times \begin{cases} Q_0 X_+ / q, & |V_+(k_y^*)| > |V_-(k_y^*)| \\ Q_0 X_- / q, & |V_-(k_y^*)| > |V_+(k_y^*)|. \end{cases} \quad (24) \end{aligned}$$

In order to obtain the left-hand side of Eq. (24) we have assumed that  $|V_+(k_y)/V_-(k_y)|$  changes slowly in the anticrossing region near  $k_y^*$ . Actually, it is clear that for the final result all that is required is that  $(|V_+(k_y)/V_-(k_y)| - 1)$  not cross zero too near to  $k_y^*$ .

Equation (24) is the basic result which we shall employ in the subsequent sections, and it is useful to assign it a

where

$$c_i^{\pm}(\vec{k}) = \frac{V}{[|V|^2 + (E_{\pm} - \epsilon_i)^2]^{1/2}}, \quad (20b)$$

$$c_{i'}^{\pm}(\vec{k}) = \frac{(E_{\pm} - \epsilon_i)}{[|V|^2 + (E_{\pm} - \epsilon_i)^2]^{1/2}}, \quad (20c)$$

$$E_{\pm} = \frac{1}{2}(\epsilon_i + \epsilon_{i'}) \pm [(\epsilon_i - \epsilon_{i'})^2 + |V|^2]^{1/2}, \quad (20d)$$

$$V = V_+(k_y) \exp(-ik_x X_+) + V_-(k_y) \exp(-ik_x X_-). \quad (20e)$$

However, to use Eq. (17) we must look at states

$$|u'_{\pm}(\vec{k})\rangle = \exp[-i\Theta_{\pm}(k_y)] |u_{\pm}(\vec{k})\rangle, \quad (21)$$

such that  $\langle u'_{\pm}(\vec{k}) | \partial u'_{\pm} / \partial k_y \rangle = 0$ . Since, within the lowest Landau level,

$$\langle u_{i'}(\vec{k}) | \partial u_i(\vec{k}) / \partial k_y \rangle = a_L^2 k_x \delta_{i',i},$$

we have

$$\frac{d\Theta_{\pm}(k_y)}{dk_y} = a_L^2 k_x + |c_i^{\pm}(\vec{k})|^2 \frac{d}{dk_y} \arg(V). \quad (22)$$

To proceed further, we assume for the sake of definiteness that  $\epsilon_{i'}(k_y) < \epsilon_i(k_y)$  for  $k_y < k_y^*$  with the inequality reversed for  $k_y > k_y^*$ . Then as  $k_y$  passes from  $k_y^{(1)} < k_y^*$  to  $k_y^{(2)} > k_y^*$ ,

$$|E_-(k_y^{(2)}) - \epsilon_i| \ll |V(k_y^{(2)})|,$$

$$|E_-(k_y^{(1)}) - \epsilon_i| \gg |V(k_y^{(1)})|,$$

and  $|u'_-(k_y)\rangle$  evolves from

$$|u_{i'}(k_y^{(1)})\rangle \text{ to } e^{-i\phi} |u_i(k_y^{(2)})\rangle,$$

where

physical interpretation. When, as a function of  $k_y$ ,

$$\langle X_{i',l}(k_y) | H | X_{i,l}(k_y) \rangle$$

crosses

$$\langle X_{i,l+1}(k_y) | H | X_{i,l+1}(k_y) \rangle,$$

it must also cross

$$\langle X_{i,l}(k_y) | H | X_{i,l}(k_y) \rangle.$$

The two possible phase shifts in Eq. (24) correspond to translations in position of the wave function of  $X_+$  when  $|V_+| > |V_-|$  and  $X_-$  when  $|V_-| > |V_+|$ . In the process of the anticrossing the electrons must, in effect, hop from  $|X_{i,l}\rangle$  to  $|X_{i',l'}\rangle$  for some value of  $l'$ . The preceding analysis establishes the physically reasonable statement that the value of  $l'$  selected is the one to which

$|X_{t,t}\rangle$  is most strongly coupled near the crossing point.<sup>16</sup> Using this notion, we can dispense with the Kubo formula and use very simple considerations to attempt evaluation of the Hall conductivity in the intra-Landau-level gaps for any periodic potential.

### III. ANISOTROPIC POTENTIAL ON A HEXAGONAL LATTICE

For a hexagonal lattice, when only the first shell of reciprocal-lattice vectors is included, the periodic potential may be written as

$$V(x,y) = V_1 \cos(Q_0 X) + V_2 \left[ \cos \left[ \frac{Q_0}{2} (x + \sqrt{3}y) \right] + \cos \left[ \frac{Q_0}{2} (x - \sqrt{3}y) \right] \right]. \quad (25)$$

$Q_0$  is related to the crystal lattice constant by  $Q_0 = 4\pi/(\sqrt{3}a)$ . (For a hexagonal crystal  $V_2 = V_1$ , but in this section we consider the case  $|V_2/V_1| \ll 1$ .) The diagonal matrix elements of the Hamiltonian in the lowest Landau level are

$$\langle X | H | X \rangle = V_1 \exp(-Q_0^2 a_L^2 / 4) \cos(Q_0 X) \equiv \epsilon_0(X), \quad (26)$$

and the off-diagonal matrix elements are

$$\langle X \pm \delta X | H | X \rangle = V_1 \exp(-Q_0^2 a_L^2 / 4) \cos[Q_0(2X \pm \delta X)/4], \quad (27)$$

where  $\delta X = \sqrt{3}Q_0 a_L^2 / 2 = 2\pi q / (pQ_0)$ . (Here  $p/q$  is the number of flux quanta per unit cell of the hexagonal lattice;  $\langle X' | H | X \rangle = 0$ , unless  $|X' - X| = \delta X$ .)

$\sigma_H$  may be evaluated either by considering an infinite system and using the Kubo formula as discussed in Sec. II, or by examining the changes in the eigenvalues spectrum of a finite system with changing magnetic field  $H$  or equivalently with changes in the undetermined constant  $\delta A$  in the vector potential. Because we consider it more physically appealing, we give an argument of the latter type. As discussed below, however, this argument can ultimately be justified only by Eq. (24), derived from the Kubo formula in the preceding section.

A given state  $|X\rangle$  is coupled, directly or indirectly to  $|X - s\delta X\rangle$  for all integral values of  $s$ . As the constant  $\delta A$  is changed all these values of  $X$  shift rigidly. For  $|V_2| \ll |V_1|$  we may take  $|X\rangle$  to be an eigenstate of  $H$  unless  $|\epsilon_0(X - s\delta X) - \epsilon_0(X)|$  goes to zero for some value of  $s$ . This can only occur for certain discrete values of  $|X\rangle$ . To see this, consider the equation

$$\cos(Q_0 X) = \cos[Q_0(X - s\delta X)] = \cos(Q_0 X - 2\pi s q / p). \quad (28)$$

This equation can be solved for some value of  $X$  only if

$$\frac{Q_0 X}{\pi} = n - \frac{s q}{p}, \quad (29)$$

for some integer  $n$ . The values of  $X$  at which this is satisfied are given, modulo  $2\pi/Q_0$ , by

$$Q_0 X = \frac{\pi k}{p}, \quad k = 1, \dots, 2p. \quad (30)$$

(This holds independent of  $q$ ; recall that  $q$  and  $p$  have no common factors.) At each of these values of  $X$  an anticrossing is created in the energy bands as a function of  $X$  when  $V_2$  is "turned-out." As is illustrated schematically in Fig. 1(a) for the case  $p/q = 3$  and in Fig. 1(b) for the case  $p/q = \frac{5}{2}$ , the states at  $|X\rangle$  and  $|X - s\delta X\rangle$  exchange places as  $\delta A$  changes so that  $X$  moves through one of these values. (Actually, these statements are somewhat simplistic and are to be understood in the sense discussed in Sec. II.) We are now in a position to determine the integer  $s$ .

Consider  $X_t \equiv (\pi + \pi t/p)/Q_0$ . This value of  $X$  is associated with the top of the  $t$ th subband of the Landau level for  $V_1 > 0$  and the bottom of the  $(p-t)$ th subband for  $V_1 < 0$ . (For example, see Figs. 1.) All the following discussions will take  $V_1 > 0$ ; the results for the hall conductivity carried by the Landau-level subbands are identical in the two cases except that the subbands appear in the opposite order in energy. It follows from Eq. (29) that

$$\frac{t - s_t q}{p} = \sigma_t, \quad (31)$$

where  $\sigma_t$  is an integer. (As we see later,  $\sigma_H = e^2 \sigma_t / h$  when the Fermi level lies in the gap above the  $t$ th subband of the Landau level.) Equation (31) determines  $s_t$  only to within a multiple of  $p$ , i.e., when  $|X_t\rangle$  is coupled to the "degenerate" state  $|X_t - s_t \delta X\rangle$  it is also coupled to  $|X_t - (s_t + kp)\delta X\rangle$  for any integer  $k$ . The effective coupling between  $|X_t\rangle$  and  $|X_t - s_t \delta X\rangle$  occurs first in  $|s_t|$ th order of perturbation theory. (These effective couplings are discussed in more detail in the next section.) We would therefore be tempted to conclude that the  $s_t$  corresponding to maximum coupling strength is the one with minimum magnitude, consistent with the requirement that  $\sigma_t$  in Eq. (31) be an integer, i.e.,  $|s_t| \leq p/2$ . (This is just the prescription found by Thouless *et al.*<sup>11</sup> for

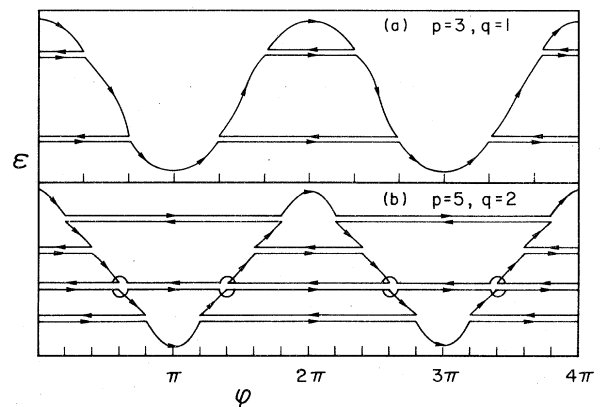


FIG. 1. Schematic illustration of the adiabatic evolution of the wave function as  $\varphi = Q_0 X$  (or equivalently  $k_y$ , or the  $y$  component of the vector potential) is changed. The arrow directions correspond to increasing  $\varphi$ .

the square-lattice case.) In our case, however, the matrix elements of  $H$  connecting  $|X_t\rangle$  with  $|X_t - 2\pi s_t q / p Q_0\rangle$  contain the factor

$$\prod_{k=\text{sgn}(s_t)}^{s_t} \cos \left[ \frac{\pi}{2} + \frac{\pi}{2p} [t - q(2k - \text{sgn}(s_t))] \right]. \quad (32)$$

This product is always nonzero when  $t+q$  is odd, and in that case we choose  $s_t$  by the requirement that  $|s_t| \leq p/2$  as in the square-lattice case. However when  $t+q$  is even, the product is zero unless

$$\mathcal{S} + 1 - p \leq s_t \leq \mathcal{S}, \quad (33a)$$

where  $\mathcal{S}$  is the smallest non-negative integer given by

$$\mathcal{S} = \frac{t-q}{2q} + N \frac{p}{q} \quad (33b)$$

for some integer  $N$ . There is a unique integer  $s_t$  in the interval defined by Eq. (33a) which yields an integral value for  $\sigma_t$ .

In Table I we list values of  $\sigma_t$  for a range of values of  $p$ ,  $q$ , and  $t$ , valid for  $|V_2/V_1| \ll 1$ . Values are listed only for  $q \leq p/2$ . It is readily demonstrated from the above prescription that when  $q$  is increased by  $p, s_{t,p,q+p} = -s_{p-t,p,q}$  which implies that  $\sigma_{t,p,q+p} = 1 - \sigma_{p-t,p,q} + s_{p-t,p,q}$ . Similarly when  $q \rightarrow p - q, s_{t,p,p-q} = s_{p-t,p,q}$

$\sigma_{t,p,p-q} = 1 - s_{p-t,p,q} - \sigma_{p-t,p,q}$ . Thus for a given  $t$  and  $p$  the quantum numbers at all values of  $q$  can be generated from those listed in Table I. (The expression given above just increase  $\sigma_{t,p,q}$  by one when  $t$  increases by  $p$ , corresponding to going from one Landau level to the next. This is not always correct for the hexagonal lattice, however, and the results given are for the lowest Landau level. Results for higher Landau levels are simply related but we do not discuss that relationship here.) All listings follow from the prescriptions given above except those for  $p$  even,  $t = p/2, q = 1$ , and  $t$  even. In that case  $s_t = \pm p/2$  both yield integral values of  $t$ , and we must go back to Eq. (32) in order to decide which value to select. It is easily verified that in all cases the magnitude of the product in Eq. (32) is larger for  $s_t = -p/2$  and thus  $\sigma_t = 1$  in all cases. Also listed in Eq. (1) are the Hall conductivity values for the square-lattice potential. The essential difference between the two potentials is that for

$$V(x,y) = V_1 \cos(Q_0 x) + V_2 \cos(Q_0 y), \quad (34)$$

Eq. (27) becomes

$$\langle X \pm \delta X | H | X \rangle = V_2/2. \quad (35)$$

The consequences of this difference may be divided into three categories.

TABLE I. Hall conductivity quantum numbers for a hexagonal crystal potential with  $|V_2/V_1| \ll 1$ .  $Ba^2\sqrt{3}/(2\Phi_0) = p/q$  is the number of the flux quanta per unit cell, and  $t$  is the number of subbands of the Landau level occupied below the Fermi level. Thus  $e^2(\sigma_t - \sigma_{t-1})/h$  is the contribution to  $\sigma_H$  from the  $t$ th subband. All these results are for  $V_1 > 0$ . For  $V_1 < 0$ , the contributions from the various subbands are unchanged but they appear in opposite order in energy. Values are given for both square ( $S$ ) and hexagonal ( $H$ ) lattices. In cases where no entry is made there is no gap and the Hall conductivity is not quantized. Cases in which the values are different are underlined. Cases in which band crossings occur are indicated by asterisks.

$\sigma_t$					$\sigma_t$					$\sigma_t$				
$q$	$p$	$t$	$S$	$H$	$q$	$p$	$t$	$S$	$H$	$q$	$p$	$t$	$S$	$H$
1	2	1		1	1	2	1	0	1	1	8	2	0	0
1	3	1	0	1	1	7	2	0	0	1	8	3	0	1
1	3	2	1	1	1	7	3	0	1	1	8	4		1
1	4	1	1	1	1	7	4	1	1	1	8	5	1	1
1	4	2		1	1	7	5	1	1	1	8	6	1	1
1	4	3	1	1	1	7	6	1	1	1	8	7	1	1
1	5	1	0	1	2	7	1	1	1	3	8	1	-1	-1
1	5	2	0	0*	2	7	2	0	2	3	8	2	1	1
1	5	3	1	1	2	7	3	1	1	3	8	3	0	3
1	5	4	1	1	2	7	4	0	0	3	8	4	-1	-1
2	5	1	1	1	2	7	5	1	1	3	8	5	1	1
2	5	2	0	2	2	7	6	0	2	3	8	6	0	0
2	5	3	1	1	3	7	1	1	1	3	8	7	2	-1
2	5	4	0	0	3	7	2	-1	-1*	1	9	1	0	1
1	6	1	0	1	3	7	3	0	3	1	9	2	0	0
1	6	2	0	0*	3	7	4	1	1	1	9	3	0	1
1	6	3		1	3	7	5	2	-1	1	9	4	0	0*
1	6	4	1	1	3	7	6	0	0	1	9	5	1	1
1	6	5	1	1	1	8	1	0	1	1	9	6	1	1

(i) For  $q=1$ ,  $p$  even, and  $t=p/2$  the effective couplings for  $s=\pm p/2$  are identical in the square-lattice potential. As a result  $\sigma_t$  is indeterminate and the corresponding gap within the Landau level closes. On the other hand, for the hexagonal potential the effective coupling for  $s=+p/2$  in this case is always smaller (it is zero for  $p/2$  odd) than that for  $s=-p/2$ , making  $\sigma=1$  for all values of  $p$ . This is the reason for the appearance of a gap at half-filling in the energy spectrum of the charge-density-wave state of electrons in a partially occupied Landau level in the hexagonal case. The gap remains closed in the square case as has been emphasized by Kuramoto.<sup>17,18</sup>

(ii) In the square-lattice potential all other values of  $\sigma_t^S$  are fixed by the requirement that  $|s_t^S| < p/2$ . The value of the Hall conductivity integer for the same  $p$  and  $q$  in the hexagonal potential  $\sigma_t^H$  is identical unless  $\sigma_t^S$  is even and  $s_t^S$  is odd. In this case  $\sigma_t^H = \sigma_t^S + q$  if  $\sigma_t^S > 0$  and  $\sigma_t^H = \sigma_t^S - q$  if  $\sigma_t^S \leq 0$ . (These statements can readily be proven from the prescription given above.) Physically these changes occur because the strongest effective coupling for the square-lattice potential, i.e., that appearing in the lowest order of perturbation theory, vanishes [a zero occurs in one of the cosine factors in Eq. (32)] for the corresponding hexagonal lattice potential.

(iii) All the discussion in this section has been for the case  $|V_2/V_1| \ll 1$ . For the square-lattice potential no gaps close and no values of  $\sigma_t$  change as a function of  $V_2/V_1$ . This statement is not a trivial one, but is justified by the following observations. The Hall conductivity may also be determined by combining Streda's formula,<sup>5,6,19,20</sup>

$$\sigma_H = \frac{e^2 \Phi_0}{hL^2} \frac{\partial N(\epsilon_F)}{\partial H}, \quad (36)$$

where  $N(\epsilon_F)$  is the number of states below the Fermi level, with a calculation of the magnetic field dependence of the electronic structure.<sup>9,21</sup> Such a calculation is available for  $V_2=V_1$  for a square-lattice potential<sup>7</sup> and leads to the same results for  $\sigma_H$  as those obtained in Ref. 11 (and here) for  $|V_2| \ll |V_1|$ .<sup>22</sup> While this does not prove that bands cannot cross and "cross back" between the two limits, no examples of such behavior have been discovered and, as see from the arguments in the next section, none are likely. On the other hand, for the hexagonal lattice, comparison via Eq. (36) with the electronic structure calculations of Claro and Wannier<sup>8</sup> shows several differences between the  $|V_2| \ll |V_1|$  and  $V_2=V_1$  situations. In the next section we show that this difference may also be directly traced to the appearance of the cosine factor in Eq. (27).

In closing this section we show that  $\sigma_H = (e^2/h)\sigma_t$  with  $\sigma_t$  defined in Eq. (31). Note that Eq. (31) implies that the Hall conductivity carried by the  $t$ th subband of the Landau level is  $(e^2/h)m_t$ , where

$$m_t = \begin{cases} \sigma_t - \sigma_{t-1} = 1/p - (s_t - s_{t-1})q/p, & t > 1 \\ \sigma_1 = 1/p - s_1 q/p, & t = 1. \end{cases} \quad (37)$$

The validity of this can be established from the Kubo formula by noting that in the  $t$ th band there are  $q$  band crossings near the band maximum, each of which, according to Eq. (24), gives a contribution to  $\sigma_H$  of  $-(e^2/h)(2\pi s_t q/p)$ .

At each gap, the development leading to Eq. (24) shows that the upper band suffers the opposite phase shift. [ $(e^2/h)(2\pi s_{t-1} q/p)$  for the  $t$ th subband]. The first term in Eq. (37) represents the classical Hall conductivity corresponding to the phase shift suffered in the absence of band crossing. Another way of obtaining the same result, which we look at as representing a physical interpretation of Eq. (24), appeals to Eq. (36). If we take the origin of coordinates at one edge (in  $x$ ) of the system, the change in vector potential  $A_y$  at the right edge of the system when  $H$  changes by  $\Delta H$  is  $L_y \Delta H$ . This corresponds to a shift of  $-L \Delta H/H$  in the center in  $X$  of a basis-set orbital with a given value of  $k_y$ . Consider  $\Delta H$  such that

$$\frac{L \Delta H}{H} = \frac{2\pi}{Q_0}. \quad (38)$$

(Note that as  $L \rightarrow \infty$  this becomes an infinitesimal change in magnetic field.) When the jumps corresponding to band crossings are taken into account a state in the  $t$ th subband of the Landau level shifts as  $|X\rangle \rightarrow |X - 2\pi m_t / Q_0\rangle$  under this change in magnetic field. Thus the change in the number of states in the  $t$ th subband is

$$\Delta N_t = \left[ \frac{2\pi p m_t}{Q_0} \right] / \left[ \frac{2\pi a_L^2}{L} \right]. \quad (39)$$

Then

$$\frac{e^2 \Phi_0}{hL^2} \frac{\Delta N_t}{\Delta H} = \frac{e^2 m_t}{h}, \quad (40)$$

as required.

#### IV. BAND CROSSINGS

We consider the set of states  $\{|X - s\delta X\rangle\}$ , where  $s$  ranges over all integers. In the hexagonal lattice potential these states are coupled together by the matrix elements

$$\begin{aligned} \langle X - (k+1)\delta X | H | X - k\delta X \rangle \\ \equiv V_{k+1,k} = V_2 \cos(-Q_0^2 a_L^2 / 4) \\ \times \cos[Q_0(X - (k + \frac{1}{2})\delta X) / 2]. \end{aligned} \quad (41)$$

We want to consider the behavior of the Greenian

$$G(\epsilon) \equiv (\epsilon - H)^{-1}, \quad (42)$$

where  $X$  is near  $X_t$  and  $\epsilon$  is near  $\epsilon_0(X_t) \equiv \epsilon_0$ . We define  $\epsilon_0(X_t - k\delta X) \equiv \epsilon_k$ . Since  $\delta X = 2\pi q / (pQ_0)$ ,  $\epsilon_k$  repeats as a function of  $k$  with period  $p$ . From Sec. III, however, there is also a degeneracy within this period  $p$ ,  $\epsilon_0 = \epsilon_{s_+} = \epsilon_{s_-}$ , where  $s_+$  ( $s_-$ ) is the smallest magnitude positive (negative) integer which gives an integral value for  $\sigma$  in Eq. (31). (Recall that  $s_+ - s_- = p$ .)

If we write

$${}^t k', k \equiv \delta_{k',k} \epsilon_k, \quad (43a)$$

$$V_{k',k} \equiv \delta_{k',k+1} V_{k+1,k} + \delta_{k',k-1} V_{k,k-1}, \quad (43b)$$

then the matrix  $\underline{V}$  is proportional to  $V_2$ . It is straightfor-

ward to generate a perturbative expansion for  $\underline{G}$  in terms of  $\underline{V}$  as

$$\underline{G}(\epsilon) = (\epsilon \underline{1} - \underline{t})^{-1} + (\epsilon \underline{1} - \underline{t})^{-1} \underline{V} (\epsilon \underline{1} - \underline{t})^{-1} + (\epsilon \underline{1} - \underline{t})^{-1} \underline{V} (\epsilon \underline{1} - \underline{t})^{-1} \underline{V} (\epsilon \underline{1} - \underline{t})^{-1} + \dots \quad (44)$$

One subsum of the terms in this expansion produces contributions to  $\underline{G}(\epsilon)$  identical to those which would be produced by the effective interaction  $V_+$  between  $|X_t\rangle$  and  $|X_t - s_t \delta X\rangle$ .  $V_+$  is defined to be  $(\epsilon - \epsilon_0)(\epsilon - \epsilon_{s_+})$  times the sum of all the contributions to  $G_{0,s_+}(\epsilon)$  in which the reciprocal of these factors appears only once, i.e.,

$$V_+ = \frac{V_{1,0} V_{2,1} \cdots V_{s_+,s_+-1}}{(\epsilon_0 - \epsilon_1)(\epsilon_0 - \epsilon_2) \cdots (\epsilon_0 - \epsilon_{s_+-1})} \times \left[ 1 + \frac{V_{2,1}^2}{(\epsilon_0 - \epsilon_1)(\epsilon_0 - \epsilon_2)} + \cdots + \frac{V_{s_+-1,s_+-2}}{(\epsilon_0 - \epsilon_{s_+-1})(\epsilon_0 - \epsilon_{s_+-2})} + O\left(\frac{V_2}{V_1}\right)^4 \right] \quad (45)$$

The terms contributing to this effective interaction correspond to hopping from  $X_0$  to  $X_{s_+}$ , taking an arbitrary number of single steps but hitting on  $X_0$  only at the start

of the path and on  $X_{s_+}$  only at the end. The effective interaction for hopping in the opposite direction,  $V_-$ , is defined similarly. Another subsum of terms in the expansion of Eq. (44) produces terms identical to those which would be produced by a shift in  $\epsilon_0$  by  $\delta\epsilon_0$ .  $\delta\epsilon_0$  is  $(\epsilon - \epsilon_0)^2$  times the contribution to  $G_{00}(\epsilon)$  from paths beginning at  $X_0$  and ending at  $X_0$  without ever crossing  $X_{s_+}$  or  $X_{s_-}$ . Thus (for  $|s_+| > 1$ ,  $|s_-| > 1$ )

$$\delta\epsilon_0 = \frac{V_{1,2}^2}{\epsilon_0 - \epsilon_1} + \frac{V_{-1,0}^2}{(\epsilon_0 - \epsilon_{-1})^2} + O\left(\frac{V_2}{V_1}\right)^4 \quad (46)$$

All matrix elements of the Greenian connecting  $X_0$  with  $X_{s_+}$ ,  $X_{s_-}$ , or  $X_0$  (and similar matrix elements with  $X_0$ ,  $X_{s_+}$ , or  $X_{s_-}$  translated by multiples of  $2\pi/Q_0$ ) are included in the terms discussed above. To determine whether  $s = s_+$  or  $s = s_-$  we need only determine whether  $|V_+| > |V_-|$ .<sup>23</sup> Including leading-order corrections we can write

$$V_{\pm} = \alpha_{\pm} \frac{V_2^{|s_{\pm}|}}{V_1^{|s_{\pm}|-1}} \left[ 1 + C_{\pm} \left(\frac{V_2}{V_1}\right)^2 + \cdots \right], \quad (47)$$

where from Eq. (45),  $\alpha_{\pm}$  is given by the product of cosines in Eq. (32). The correction factor  $C_{\pm}$  comes partly from the correction terms in Eq. (45) and partly from the effect of the energy shifts in Eq. (46) on the leading term in Eq. (45). Hence,

$$C_{\pm} = \left(\frac{V_1}{V_2}\right)^2 \left[ \sum_{k=\text{sgn}(s_{\pm})}^{\text{sgn}(s_{\pm})(s_{\pm}-2)} \frac{V_{k+1,k}^2}{(\epsilon_0 - \epsilon_k)(\epsilon_0 - \epsilon_{k+1})} - \left(\frac{V_{0,1}^2}{\epsilon_0 - \epsilon_1} + \frac{V_{0,-1}^2}{\epsilon_0 - \epsilon_{-1}}\right) \sum_{k=\text{sgn}(s_{\pm})}^{\text{sgn}(s_{\pm})(s_{\pm}-1)} \frac{1}{\epsilon_0 - \epsilon_k} \right] \quad (48)$$

TABLE II. Band crossings predicted by Eqs. (49) with  $|V_{\text{cr}}/V_1| < 1$ ,  $|C_+ V_{\text{cr}}^0/V_1^2| < 0.5$ , and  $|C_-(V_{\text{cr}}^0/V_1)^2| < 0.5$ .  $V_{\text{cr}}^*$  is the value of  $V_2$  at which the crossing actually occurs; if no crossing occurs  $V_{\text{cr}}^*$  is listed as NC.  $\sigma_t$  is the Hall conductivity in the gap for  $V_2 < V_{\text{cr}}^*$  and  $\sigma_t'$  is the value for  $V_2 > V_{\text{cr}}^*$ .

$q$	$p$	$t$	$V_{\text{cr}}^0/V_1$	$V_{\text{cr}}/V_1$	$V_{\text{cr}}^*/V_1$	$\sigma_t(\sigma_t')$
1	5	2	0.2639	0.2758	0.2789	0(1)
1	6	2	0.6563	0.7220	1.0000	0(1)
3	7	2	0.1918	0.1958	0.1962	-1(2)
1	9	4	0.0282	0.0282	0.0282	0(1)
4	9	3	0.6201	0.6971	0.7579	-1(3)
1	10	4	0.2171	0.2220	0.2225	0(1)
3	10	2	0.5168	0.5296	0.5438	-1(2)
1	11	4	0.4300	0.4526	0.4590	0(1)
3	11	4	0.1278	0.1289	0.1290	-1(2)
4	11	5	0.5203	0.6025	0.6187	-1(3)
5	11	8	0.4067	0.3089	0.3522	3(-2)
1	13	6	0.0028	0.0028	0.0028	0(1)
3	13	2	0.7103	0.7260	0.7263	-1(2)
4	13	3	0.8053	0.8296	NC	-1(1)
4	13	11	0.0721	0.0731	0.0732	-1(3)
5	13	4	0.1084	0.1092	0.1092	-2(3)
1	14	6	0.0683	0.0685	0.0685	0(1)
3	14	4	0.4474	0.4616	0.4691	-1(2)
1	15	6	0.1991	0.2027	0.2040	0(1)
4	15	5	0.7324	0.7659	0.8600	-1(3)
4	15	13	0.0557	0.0564	0.0565	-1(3)
7	15	4	0.0180	0.0180	0.0180	-3(4)

As mentioned in Sec. III, if  $t+q$  is even either  $\alpha_+$  or  $\alpha_-$  is zero and the ratio  $|V_+/V_-|$  cannot cross one as a function of  $V_2/V_1$ . For these cases no band crossings should be expected as a function of  $V_2/V_1$ , and the previous prescription for determining  $\sigma_t$  should remain correct. On the other hand, for  $t+q$  odd, neither  $\alpha_+$  nor  $\alpha_-$  is zero. In this case  $s = s_<$  [where  $s_<$  ( $s_>$ ) is the integer of

lesser (greater) magnitude between  $s_+$  and  $s_-$ ] when  $V_2 \ll V_1$ . However, if  $|\alpha_>| > |\alpha_<|$  there is a possibility of a band crossing and associated conductivity change as a function of  $V_2/V_1$ . By setting  $|V_+| = |V_-|$  this crossing should occur at  $V_2 = V_{cr}$ , where

$$V_{cr} = V_{cr}^0 \left[ 1 + \frac{C_> - C_<}{|s_>| - |s_<|} \left( \frac{V_{cr}^0}{V_1} \right)^2 + \dots \right] \quad (49a)$$

and

$$V_{cr}^0 = V_1 \left| \frac{\alpha_<}{\alpha_>} \right|^{1/(|s_>| - |s_<|)} \quad (49b)$$

The problem with applying this analysis is that it is difficult to know *a priori* whether or not the perturbative treatment is still valid at the value of  $V_2$  at which the crossing is predicted to occur. We have been unable to devise a criterion which both predicts all crossings which occur and which predicts no crossings which do not occur. Nevertheless, we find that the bulk of the crossings are quite well described in the preceding analysis. For example, we can fairly arbitrarily decide to accept all predicted crossing values with  $|V_{cr}/V_1| < 1$ ,  $|C_+(V_{cr}^0)/V_1|^2 < 0.5$ , and  $|C_-(V_{cr}^0)/V_1|^2 < 0.5$ . This leads to a prediction of crossings for  $p \leq 15$  at the values of  $q \leq p/2$ , listed in Table II. In all, out of about 300 cases band crossings are predicted to occur 22 times.<sup>24</sup> When checked by an explicit calculation of the energy gap as a function of  $V_2/V_1$ , 21 of these predicted crossings are found to occur, usually at values of  $V_2$  very close to those predicted in Eq. (49). A more restrictive criterion for the validity of the perturbative analysis would eliminate incorrect predictions of crossings, but would miss some of the crossings listed in Table II. We do not believe that any crossings occur for  $p \leq 15$  and  $|V_{cr}/V_1| < 1$ , other than those listed in Table II. In all the cases listed when  $V_2$  crosses  $V_{cr}^*$ ,  $s_t$  changes from the minimum magnitude possible value to the minimum magnitude among possible values of the opposite sign. As a result  $\sigma_t$  suddenly changes by  $q$ . Most often the change is such that  $\sigma_t$  increases; this may be traced to the fact that  $\cos[Q_0(X_t + s\delta X)/2]$  is generally larger in magnitude for positive values of  $s$  [see Eq. (27)]. For the square-lattice potential, this cosine factor does not appear [see Eq. (35)] and we have checked that no crossings are predicted by Eqs. (49), using the criteria of Table II, at least up to  $p = 50$ .

In Figs. 2(a) and 2(b), we have plotted some band gaps as a function of  $V_2/V_1$ . For the cases plotted in Fig. 2(a) no crosses occur. One can easily verify that the gaps follow the expected power-law behavior,

$$E_g \sim |V_>| \sim V_1 \left| \frac{V_2}{V_1} \right|^{|s_>|}, \quad (50)$$

over wide ranges of  $V_2/V_1$ . For the cases plotted in Fig. 2(b), band crossings occur. These curves still follow power-law behavior for  $V_2/V_1 \ll 1$ , but deviate as the band crossing approaches. Some curves show renewed power-law behavior after the crossing, but with a new power corresponding to the changed value of the quantum number  $s_t$  in the gap. Several of the curves also show ad-

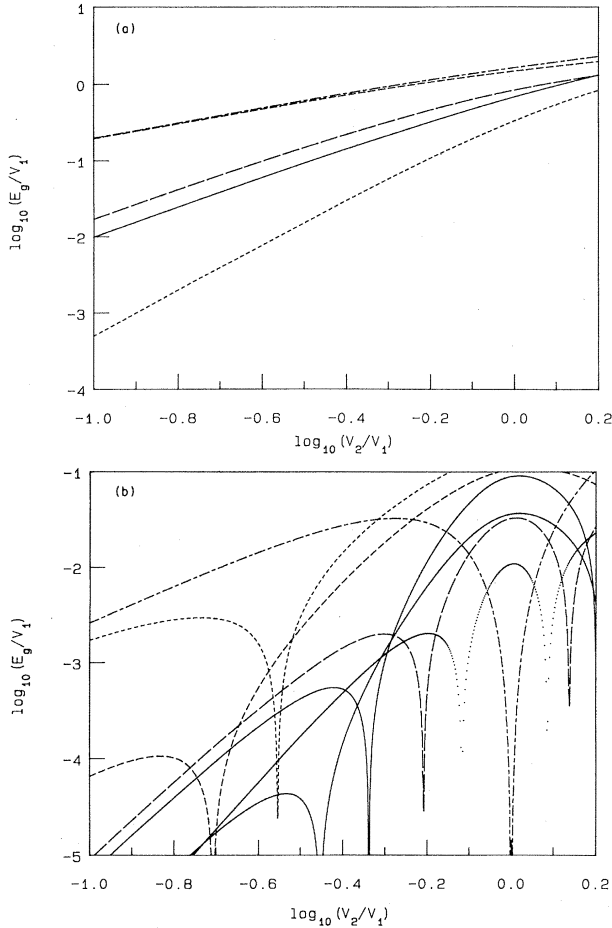


FIG. 2. (a) Band gaps as a function of  $V_2/V_1$  for the hexagonal lattice potential.  $E_g$  is the gap divided by  $\exp(-Q_0^2 a_L^2/4)$ . (Solid line  $t=1$ ,  $q/p = \frac{1}{3}$ ; short-dashed line  $t=1$ ,  $q/p = \frac{1}{4}$ ; short-dashed-long-dashed curve  $t=3$ ,  $q/p = \frac{1}{4}$ ; medium-dashed line  $t=2$ ,  $q/p = \frac{1}{3}$ ; long-dashed line  $t=2$ ,  $q/p = \frac{1}{4}$ ). Note that the gaps approximately follow power-law behavior as a function of  $(V_2/V_1)$  with the exponent in agreement with the value given for  $s_t$  in Table I. (b) This figure illustrates some cases in which the gaps close as a function of  $V_2/V_1$ . [Some curves show a finite minimum value for  $\log_{10}(V_2/V_1)$  which reflects only the finite set of  $(V_2/V_1)$  values used to generate the curves for this illustration.] [Solid lines  $t=4$ ,  $q/p = \frac{1}{11}$ , for which  $\log_{10}(V_{cr}^*/V_1) = -0.338$  and  $t=8$ ,  $q/p = \frac{5}{11}$  for which  $\log_{10}(V_{cr}^*/V_1) = -0.555$ ; short-dashed-long-dashed curve  $t=2$ ,  $q/p = \frac{1}{6}$ , for which  $\log_{10}(V_{cr}^*/V_1) = 0$ ; medium dashed line  $t=2$ ,  $q/p = \frac{3}{7}$ , for which  $\log_{10}(V_{cr}^*/V_1) = -0.707$ ; long dashed line  $t=5$ ,  $q/p = \frac{4}{11}$ , for which  $\log_{10}(V_{cr}^*/V_1) = -0.209$ ; dotted line  $t=2$ ,  $q/p = \frac{3}{13}$ , for which  $\log_{10}(V_{cr}^*/V_1) = -0.118$ .] Several curves show additional band crossings which occur for  $V_2/V_1 > 1$ .



ditional band crossings at  $|V_2/V_1| > 1$ , which are not predicted by the perturbative analysis.

### V. SUMMARY AND CONCLUDING REMARKS

We have derived, starting from the Kubo formula, a very simple and physically transparent criterion for determining the Hall conductivity in intra-Landau-level gaps for electrons in a strong magnetic field and a weak periodic potential. This criterion has been applied here to the case of hexagonal periodic potential and has been shown to provide a clear account of the physical origin of the substantial differences between this case and that of the

square-lattice potential. In contrast to numerical calculations starting directly from the Kubo formula,<sup>12</sup> the result for  $\sigma_H$  is almost apparent by inspection. The same criterion can be used with equal simplicity for other periodic potentials and also to study the dependence of  $\sigma_H$  in a gap on magnetic field.<sup>25</sup>

### ACKNOWLEDGMENTS

The author would like to thank Professor D. J. Thouless and Dr. D. Yoshioka for some very useful comments on a previous version of this manuscript, and particularly for bringing Ref. 8 to his attention.

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<sup>9</sup>A. H. MacDonald, Phys. Rev. B **28**, 6713 (1983).

<sup>10</sup>If  $BA_0/\phi_0$  is irrational, the so-called irrational fields, the energy spectrum may be singular continuous.

<sup>11</sup>D. J. Thouless, M. Kohmoto, M. P. Nightingale, and M. den Nijs, Phys. Rev. Lett. **49**, 405 (1982).

<sup>12</sup>D. Yoshioka, Phys. Rev. B **27**, 3637 (1983).

<sup>13</sup>The restriction to the lowest Landau level becomes valid when  $\hbar\omega_c \gg |V_{n,m}|$ . To examine the magnetic field dependence of the spectrum the basis set must include the corresponding magnetic Bloch functions for each Landau level, but  $k_x$  and  $k_y$  remain good quantum numbers. The magnetic field dependence of the energy spectrum and of the Hall conductivity is discussed elsewhere [A.H. MacDonald (unpublished)].

<sup>14</sup>The velocity operators have no matrix elements between different values of  $\vec{k}$ .  $\{u_\alpha(\vec{k}), \epsilon_\alpha(\vec{k})\}$  is the set of all eigenfunctions and eigenvalues of  $H_{\text{eff}}(\vec{k})$ , including those from all Landau levels.

<sup>15</sup>In periodic potentials each Landau level is split into  $p$  nonoverlapping subbands. On the other hand the number of band in-

trices per Landau level [ $j$  in Eq. (9)] can be greater than  $p$  for a general potential. For example, in the hexagonal case  $j = 2p$  if  $q$  is odd. In this case the bands must go together in groups of  $j/p$ , and crossings are possible within a group but not between groups. It is possible however to work with a single analytic function of  $\vec{k}$  for each subband in an "extended" Brillouin zone in which  $k_x \in [0, Q_0/q]$ .

<sup>16</sup>In our analysis we included only the coupling to the values of  $X_{i,l}$  which are adjacent to  $X_{i,l}$ , but this statement can be generalized.

<sup>17</sup>Y. Kuramoto and R. R. Gerhardts, J. Phys. Soc. Jpn. **51**, 3810 (1982).

<sup>18</sup>Y. Kuramoto, Phys. Rev. Lett. **50**, 866 (1983).

<sup>19</sup>A. Widom, Phys. Lett. **90A**, 474 (1982).

<sup>20</sup>P. Středa and L. Smrčka, J. Phys. C **16**, L895 (1983).

<sup>21</sup>P. Středa, J. Phys. C **15**, L1299 (1982).

<sup>22</sup>If there are no crossings for  $|V_2/V_1| \in (0,1)$ , there can be none for  $|V_2/V_1| \in (1, \infty)$ , since  $V_2$  and  $V_1$  can be interchanged by a rotation of the coordinate system.

<sup>23</sup>As mentioned previously for the hexagonal lattice potential, if  $q$  is odd, effective off-diagonal couplings change sign when  $X$  and  $X'$  are shifted by  $2\pi q/Q_0$ , i.e., when  $k \rightarrow k + p$ . However, only  $|V_+/V_-|$  enters the criterion for determining  $s$ , and we need not take explicit account of the different periodicities in  $X$  for diagonal and off-diagonal matrix elements. This would not be true for general periodic potentials.

<sup>24</sup>A list of crossings predicted on the basis of Eq. (49) up to  $p = 50$  is available from the author.

<sup>25</sup>A. H. MacDonald (unpublished).