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On the energy spectrum of lateral surface superlattices in a magnetic field: influence of Landau level coupling

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Abstract. A numerical investigation of the single-particle energy spectrum of two-dimensional electrons subject to a periodic potential of square symmetry and a perpendicular magnetic field is presented. Our approach allows variation of both the steepness and the strength of the modulation potential. It is shown that the inclusion of coupling between different Landau levels has a strong impact on the appearance of the subband structure. The possibility of finding experimental indications of the spectrum is discussed in the light of the present calculations.

1. Introduction

The problem of Bloch electrons in a magnetic field has attracted renewed interest in recent years. The remarkable advent of nano-fabrication techniques made it possible to create two-dimensional lateral surface superlattices with modulation periods much shorter than the elastic mean free path and comparable to the cyclotron radius at low magnetic fields. The self-similar single-electron energy spectrum of such a system in a perpendicular magnetic field is the famous 'Hofstadter butterfly' [1]. The characteristic subband structure of the Landau levels has been resolved, indirectly, as a suppression of the band conductivity in low-temperature transport measurements on modulated GaAs structures by Weiss *et al* [2]. This purely quantum mechanical effect was successfully described by Gerhardts *et al* [3, 4], who found that the relative contributions to the total conductivity from the band conductivity and the scattering conductivity are determined by the relation between the collision broadening and the modulation broadening of the energy spectrum. The underlying assumption of weak modulation that allows the neglect of coupling between different Landau levels in their theory is certainly fulfilled under the experimental conditions of [2]. For stronger modulation, however, this approximation is expected to fail.

In the present paper we consider the influence of interaction among the Landau levels (LLs) on the energy spectrum with increasing modulation amplitude V_0. Qualitatively, one expects a broadening of free LLs until magnetic breakdown takes place when the Landau bandwidth is approximately equal to the free LL spacing [5]. Further increase of V_0 results in a situation where the lattice effects are dominant: the subbands cluster in distinct energy bands resembling the well known spectrum of the Mathieu equation for zero magnetic field (Onsager regime). While these effects were studied some time ago for simple sinusoidal

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potentials and for certain flux ratios per unit cell ('pure cases') [6, 7], only recently has work appeared attempting to include LL coupling within an extended version of Harper's equation for arbitrary rational fluxes [8, 9] as well as within an approach based on the use of symmetry adapted basis functions [10]. Such a generalization is desirable for two reasons. First, there is growing interest in experiments on strongly modulated systems, i.e. on anti-dot arrays [11]. Second, the explanation of the magneto-transport measurements in terms of classical chaotic dynamics [12] suggests a potential much steeper than a cosine. In addition, self-consistent screening of the periodic perturbation by the two-dimensional electron gas (2DEG) is known to enhance the relative importance of higher harmonics [13], which have to be included for larger modulation amplitudes.

The outline of our approach has been published previously in detail [14] and will be summarized briefly in the next section. Typical numerical results are presented and discussed in section 3. Finally, we draw some conclusions on the conditions under which the spectrum might be observable.

2. Outline of the theory

We consider a 2DEG in the plane $z = 0$ subject to a periodic modulation potential of square symmetry with fixed period a and amplitude V_0:

$$V_N(x, y) = V_0[\cos(Kx/2)\cos(Ky/2)]^{2N} \tag{1}$$

where $K = 2\pi/a$. Obviously, the larger the integer N ($N = 1, 2, \ldots$) the steeper is the resulting potential.

The application of a perpendicular magnetic field reduces the translation symmetry of the system. Nevertheless, for magnetic fields B such that the flux per unit cell is a rational multiple of the flux quantum $\Phi_0 = h/e$, the eigenstates of the Hamiltonian may be classified by the eigenvalues of magnetic translation operators [15]. This condition reads $\alpha = Ba^2/\Phi_0 = p/q$ with p and q integers prime to each other. For the diagonalization of the full Hamiltonian, including the vector potential $A = (0, Bx, 0)$ in Landau gauge and the scalar potential (1), the wavefunctions are expanded into the symmetry adapted basis set [16]

$$\phi_{\nu,m,k}(x, y) = M_x^{-1/2} \sum_{s=-\infty}^{+\infty} \exp[-ik_x l_m^2 (sp + m) K_y] \Psi_{\nu,k_y+(sp+m)K_y}(x, y). \tag{2}$$

Here, $\Psi_{\nu,k_y}(x, y) = \exp(ik_y y) u_\nu(x - k_y l_m^2)$ is the solution of the free particle Hamiltonian with properly normalized oscillator function $u_\nu(x)$, M_x is the number of magnetic unit cells in the x direction, and $l_m = (\hbar/eB)^{1/2}$ is the magnetic length. The allowed k vectors ($k = (k_x, k_y)$) are now restricted to the first magnetic Brillouin zone (MBZ), i.e., $|k_x| \leqslant \pi/qa$ and $|k_y| \leqslant \pi/a$. Modulation induced gaps on the zone boundaries appear: each LL splits into p subbands of equal weight. In the resulting linear matrix eigenvalue problem

$$\sum_{\nu\nu'} \sum_{mm'} A^k_{\nu'm'} [(E_\nu - \bar{\epsilon})\delta_{\nu\nu'}\delta_{mm'} + V^{mm'}_{\nu\nu'}(k)] = 0 \tag{3}$$

the summation runs only over reciprocal lattice vectors with $m = 1, \ldots, p$. The matrix elements $V_{\nu\nu'}^{mm'}(\boldsymbol{k})$ have been calculated previously [14] for arbitrary N; the results are summarized in the appendix. $E_\nu = \hbar\omega_c(\nu + \frac{1}{2})$ is the energy of the νth LL ($\omega_c = eB/m^*$), and $\tilde{\epsilon} = \epsilon - 2^{-4N}V_0C_{NN}$ (ϵ is the eigenvalue to be determined).

In principle, the Hamiltonian matrix contains interactions of all LLs, which broaden due to the presence of the periodic potential. To obtain an idea about the order of magnitude of V_0 for which the Landau bands approach each other for a certain k we consider two adjacent Landau bands for $\alpha = 1$ and neglect their mutual repulsion in the first place. Then, they will cross for

$$V_{\nu\nu}^{11}(\boldsymbol{k}) - V_{\nu+1\nu+1}^{11}(\boldsymbol{k}) = \hbar\omega_c.$$

It should be noted that occasionally the bands may not actually cross but overlap for different $\boldsymbol{k}$ vectors, which is of no importance here. Keeping only the dominant $i = j = N-1$ term of the summation in the matrix element (A1) yields

$$\frac{\hbar^2K^2}{2m^*} \simeq \frac{V_0}{2^{4N-1}}\exp(-\pi/2)\pi\left\{C_{N-1,N}[\cos(ak_y) + \cos(ak_x)][L_\nu(\pi) - L_{\nu+1}(\pi)]\right.$$
$$\left. - C_{N-1,N-1}\cos(ak_y)\cos(ak_x)\exp(-\pi/2)[L_\nu(2\pi) - L_{\nu+1}(2\pi)]\right\}. \qquad (4)$$

Here we have used the fact that, by definition, $\hbar\omega_c = (\hbar^2K^2/2m^*)(\alpha/\pi)$. Since we have fixed the magnetic flux here it seems to us natural to express the relevant energy in terms of the crystal momentum [1]. The RHS of this relation results from the lowest order approximation of the non-interacting modulation broadened Landau bands. In this approximation, the dependence on V_0 is linear. With increasing N the breakdown condition is fulfilled for lower V_0 already since the numerical factors C_{ij} (A2) grow rapidly. Despite the fact that this estimation is valid only for unit flux ratio this behaviour is more general since the Landau bands are more dispersive for higher N [14].

A qualitative understanding of the interplay between potential steepness and LL coupling for arbitrary α and N can be achieved by examining the term (A6) in $V_{\nu\nu'}^{mm'}(\boldsymbol{k})$ which is mainly responsible for the bandwidth:

$$D_{\nu'\nu}^{rs} \simeq \exp(-W_{rs}/2\alpha)\left(\frac{W_{rs}}{\alpha}\right)^{\xi/2}L_{\nu_l}^{\xi}\left(\frac{W_{rs}}{\alpha}\right). \qquad (5)$$

Here, the steepness enters via the function $W_{rs} = \pi(r^2 + s^2)$; r and s are equivalent to the order of the Fourier components on the lattice for a given N. LL coupling comes into play via $\xi = |\nu' - \nu|$, which gives the energetic difference between the LLs under consideration. Due to the exponential in (5) higher harmonics influence the spectrum for large α only, i.e. for large magnetic field strengths. On the other hand, for large enough fields a decoupling of the LLs is possible. The relation between these two aspects becomes clear now from (5): the smaller the ratio $W_{rs}/2\alpha$, the more effective becomes a certain Fourier component of the potential. Since $(W_{rs}/\alpha)^{\xi/2}$ goes rapidly to zero then with increasing ξ (i.e. for more distant LLs) we can expect that both higher-order Fourier components and LL coupling are of importance in an intermediate range, $W_{rs} \gtrsim \alpha$.

3. Results and discussion

Our numerical analysis was carried out for GaAs based structures ($m^* = 0.067m_0$) with lattice constants of $a = 200$ nm, typical for experiments [2]. This means that $\hbar\omega_c \simeq 0.2$ meV for $\alpha = 1$.

In figures 1 and 2 we show the dependence of the Landau bands on the potential strength V_0 for a fixed flux ratio of $1/\alpha = \frac{1}{2}$. In the weak coupling limit, each Landau band consists of two subbands. Increasing V_0 leads to a crossover from this Landau regime to the so called Onsager regime, where the magnetic field causes only a weak perturbation of the potential [6]. Between these two limits there exists a region of magnetic breakdown, where inter-band (Zener) tunnelling is likely to occur [5]. The detailed behaviour, however, reveals a strong dependence on the shape of the potential as can be seen by comparing figure 1 ($N = 1$) with figure 2 ($N = 3$). The more dispersive Landau bands for the steeper ($N = 3$) potential are reaching the breakdown regime (compare (4) and the Onsager regime at a lower potential strength compared to the $N = 1$ case. It should be mentioned that the gaps between the subbands as well as those between different Landau bands do not completely vanish although their widths are below the resolution of the graphs in some cases. The level crossings are actually replaced by anti-crossings in the interacting multi-band system.

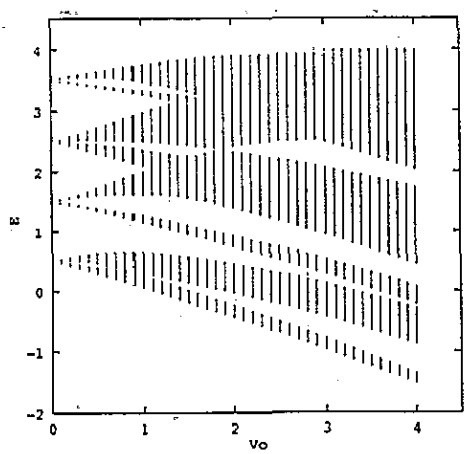

Figure 1. Landau band structure for $1/\alpha = 1/2$ and $N = 1$ as a function of the potential strength V_0. The crossover from nearly free LLs to the magnetic breakdown region is discussed in the text. The number of LLs necessary to obtain numerical convergence was about 25. The scaled energy used throughout the figures is $E = \tilde{\epsilon}/\hbar\omega_c$.

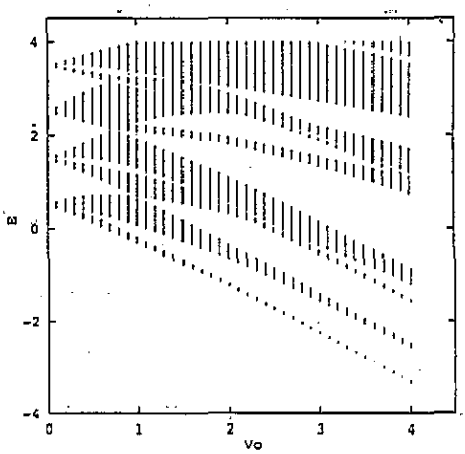

Figure 2. The same as in the previous figure but for a steeper potential with $N = 3$. The more dispersive character of the Landau subbands compared with figure1 is obvious.

Figures 3–6 show four representative spectra with their full flux ratio dependence. Figure 3 shows the spectrum for an $N = 1$ potential with $V_0 = 0.5$ meV. While the LLs are still well separated for these parameters the modification of the internal subband structure within each Landau band compared with the spectra for the uncoupled case in [14] is apparent. Increasing the potential strength to $V_0 = 1.0$ meV in figure 4 leads to a further change of the subband structure due to the fact that the Landau bands tend to touch each other if (4) holds. Even though the gaps in the third Landau band are becoming very small the large gap in the second Landau band survives.

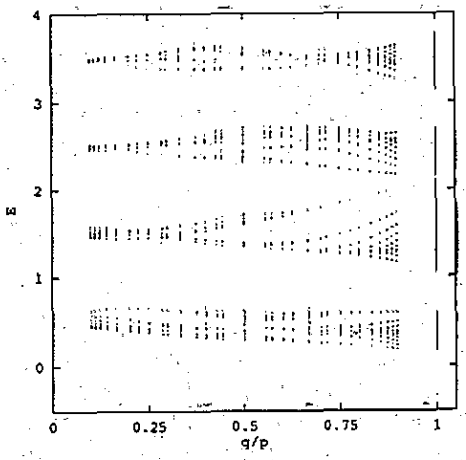

Figure 3. Energy spectrum for a potential with $N = 1$ and a strength of $V_0 = 0.5$ meV. The calculations of the spectrum were carried out up to a maximum depth of $p = 10$ throughout the remaining figures.

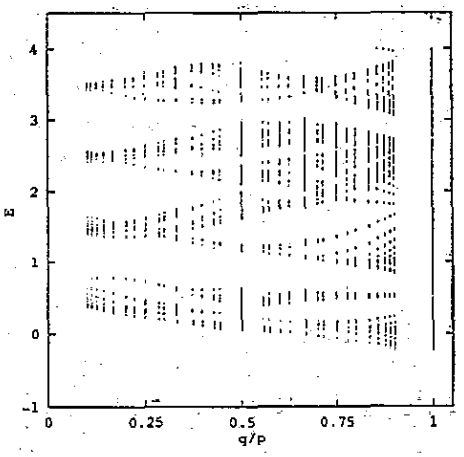

Figure 4. Spectrum for the $N = 1$ potential and an increased modulation amplitude of $V_0 = 1$ meV.

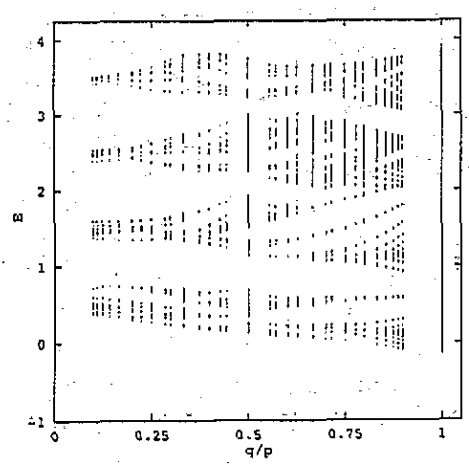

Figure 5. The same as in figure 3 but for $N = 3$. This steeper potential causes a stronger coupling (see text). Some of the gaps due to anti-crossing between LLs are below the resolution of the graph.

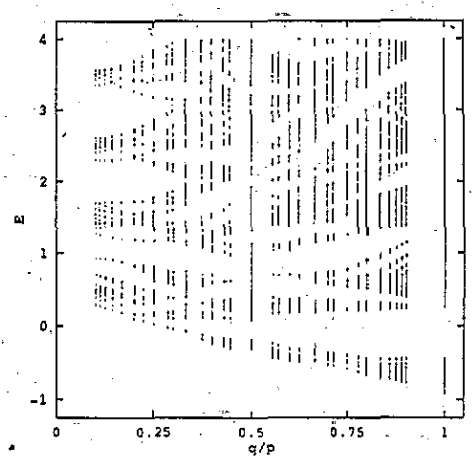

Figure 6. The case $V_0 = 1$ meV and $N = 3$. Most remarkable is the behaviour of the lowest Landau band. The large gap in the lowest Landau band survives even in the region of strong LL coupling.

From (4) a drastic alteration can be expected if one increases the power of the potential in (1) while keeping V_0 constant. This is shown for $N = 3$ in figure 5 ($V_0 = 0.5$ meV) and figure 6 ($V_0 = 1.0$ meV). Looking at figure 6 we note some interesting features for this highly coupled case. The tendency observed in figure 4 continues: while most of the gaps shrink in the region of strong coupling some of them remain in the spectra. These gaps may even extend over several Landau bands. In addition we note the large gap within the lowest Landau band. Interestingly, its upper part tends to merge with the first Landau band while the lower branch seems to be repelled. Because of the lack of a neighbouring band on the low-energy side there is a prominent gap in the lowest Landau band ranging from

$1/\alpha = \frac{1}{4}$ to $1/\alpha = 1$. The formation of large gaps even in the region of strong coupling can already be anticipated from figures 1 and 2: we note that the ranges of V_0 values where the broadened LLs approach each other (for $\alpha = 1$ roughly given by (4)) depend on the subband indices. Although these two figures are for a particular α there is a more or less smooth dependence of the subband structure on the flux ratio that becomes obvious now from figure 6.

4. Conclusions

In summary, we have investigated the single-particle energy spectrum in an artificial 2D periodic potential and a perpendicular magnetic field. With the chosen form of the potential we were able to discuss the influence of the steepness as well as the strength of the modulating potential on the spectrum for arbitrary rational flux ratios. It was shown that coupling between different Landau levels causes a strong modification of the spectra compared to the ideal Hofstadter case even for parameters that are easily met in current measurements. These coupling effects are more significant for steeper (anti-dot like) potentials. We have discussed that the importance of LL interactions is mainly determined by the relation between potential amplitude and cyclotron energy and by the Landau index ν. It should be noted that in the experiments there are usually several LLs occupied. Nevertheless, our results indicate that some features of the self-similar band structure, such as the field dependent modulation of the bandwidth and the presence of gap regions, should be observable under realistic conditions.

Finally, we should mention that while considering the aspect of modulation broadening we did not analyse other effects such as the disorder broadening of the Hofstadter spectrum which is of equal importance for an experimental observation. A detailed analysis of the influence of different kinds of disorder, however, was given recently by Wulf and MacDonald [17].

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Appendix

The matrix elements of the potential (1) are:

$$V_{\nu\nu'}^{mm'}(k) = \frac{V_0}{2^{4N}} \exp(-\mathrm{i}k_x a(m-m')/\alpha) \times \sum_{i,j=0}^{N-1} [C_{iN} A_1(N-i,0) + C_{jN} A_2(0,N-j) + C_{ij} A_3(N-i,N-j)] \quad \text{(A1)}$$

with numerical factors

$$C_{ij} = \binom{2N}{i}\binom{2N}{j}. \quad \text{(A2)}$$

The functions A_i are given by

$$A_1(r,s) = D^{rs}_{\nu'\nu} T^r_m \delta_{mm'} \tag{A3}$$
$$A_2(r,s) = D^{rs}_{\nu'\nu}\{\delta_{m-m',s}[\mathrm{sgn}(\nu'-\nu)]^\xi + \delta_{m-m',-s}[\mathrm{sgn}(\nu-\nu')]^\xi\}$$

and

$$A_3(r,s) = D^{rs}_{\nu'\nu}\{[\mathrm{sgn}(\nu'-\nu)]^\xi \delta_{m-m',s}\cos[\Theta^{m'}_{rs}(\nu',\nu)] + [\mathrm{sgn}(\nu-\nu')]^\xi \delta_{m-m',-s}\cos[\Theta^{m}_{rs}(\nu,\nu')]\} \tag{A4}$$

with the angle

$$\Theta^m_{rs}(\mu',\mu) = r[k_y a + 2\pi(m+s/2)]/\alpha + \mathrm{sgn}(\mu'-\mu)\xi \tan^{-1}(r/s). \tag{A5}$$

As a consequence of the periodicity with respect to p, the Kronecker delta in (A3)–(A4) is defined as follows: $\delta_{m-m',s} = 1$ if $m - m' = s$ and if $m - m' + p = s$; otherwise it gives zero. The function $D^{rs}_{\nu'\nu}$ reads

$$D^{rs}_{\nu'\nu} = \left(\frac{\nu_1!}{\nu_2!}\right)^{1/2} \exp(-W_{rs}/2\alpha)\left(\frac{W_{rs}}{\alpha}\right)^{\xi/2} L^\xi_{\nu_1}\left(\frac{W_{rs}}{\alpha}\right) \tag{A6}$$

with $W_{rs} = \pi(r^2+s^2)$, $\xi = |\nu - \nu'|$, $\nu_1 = \min(\nu,\nu')$, and $\nu_2 = \max(\nu,\nu')$; $L^a_n(x)$ is the associated Laguerre polynomial.

Finally, T^r_m was introduced as

$$T^r_m = \pm 2\cos[r(k_y a + 2\pi m)/\alpha] \tag{A7}$$

for ξ even (+ (−) if $\xi = 4M$ ($\xi = 4M+2$)), whereas

$$T^r_m = \mp 2\sin[r(k_y a + 2\pi m)/\alpha] \tag{A8}$$

holds for ξ odd (− (+) if $\xi = 4M+1$ ($\xi = 4M+3$)), with M an integer. This function corresponds to the cosine term in Harper's equation if one considers the simplest additive potential form.

References

[1] Hofstadter D R 1976 *Phys. Rev.* B **14** 2239
[2] Weiss D, Menschig A, von Klitzing K and Weimann G 1992 *Surf. Sci.* **263** 314
[3] Gerhardts R R, Weiss D and Wulf E 1991 *Phys. Rev.* B **43** 5192
Gerhardts R R and D Pfannkuche 1992 *Surf. Sci.* **263** 324
[4] Pfannkuche D and Gerhardts R R 1992 *Phys. Rev.* B **46** 12606
[5] Fischbeck H J 1970 *Phys. Status Solidi* b **38** 11 and references cited therein
[6] Neumann H W and Rauh A 1979 *Phys. Status Solidi* b **96** 233
[7] Schellnhuber H J and Obermair G M 1980 *Phys. Rev. Lett.* **45** 276
[8] Petschel T and Geisel T 1993 *Phys. Rev. Lett.* **71** 239
[9] Wu X and Ulloa S E 1993 *Phys. Rev.* B **47** 10028
[10] Silberbauer H 1992 *J. Phys.: Condens. Matter* **4** 7355
[11] Lorke A 1992 *Surf. Sci.* **263** 307
[12] Fleischmann R, Geisel T and Ketzmerick R 1992 *Phys. Rev. Lett.* **68** 1367
[13] Gerhardts R R 1992 *Phys. Rev.* B **45** 3449
[14] Kühn O, Fessatidis V, Cui H L, Selbmann P E and Horing N J M 1993 *Phys. Rev.* B **47** 13019
[15] Landau L D and Lifshitz E M *Theoretical Physics* vol 9 (Berlin: Akademie) p 250
[16] Thouless D J, Kohmoto M, Nightingale M P and den Nijs M 1982 *Phys. Rev. Lett.* **49** 405
Usov N A 1988 *Sov. Phys.–JETP* **67** 2565
[17] Wulf U and MacDonald A H 1993 *Phys. Rev.* B **47** 6566