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1993 J. Phys.: Condens. Matter 5 5437

(http://iopscience.iop.org/0953-8984/5/31/008)

J. Phys.: Condens. Matter 5 (1993) 5437–5442. Printed in the UK

Superlattice surface states in external fields

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Received 14 October 1992, in final form 25 March 1993

Abstract. The influence on superlattice surface states of a magnetic field $\boldsymbol{B}$ parallel to the interfaces and of a crossed electric field $\boldsymbol{F}$ and magnetic field $\boldsymbol{B}$ is considered theoretically. The degeneracy of the surface states is shown to be lifted in the magnetic field, and a picture of interaction with bulk levels in this case is given. In crossed fields the energy levels have a characteristic anticrossing behaviour as functions of B as well as F. Comparison of electric and magnetic quantization is performed.

The influence of electric and magnetic fields on solids has been the subject of extensive investigations since the early days of quantum mechanics. Recent advances in semiconductor technology allow one to build up nanostructures with previously predicted parameters. This stimulates further theoretical research on phenomena taking place in micro-objects. One interesting problem is the surface effects which result from interruption of the periodic potential of the crystal. Recently surface states which were predicted long ago by Tamm [1] were observed experimentally in superlattices (SLs) [2, 3]. This renewed theoretical interest in this quantum-mechanical phenomenon [4–8]. Earlier the surface state behaviour in external electric fields was studied extensively in connection with field-ion microscopy (see, e.g., [9, 10], and references therein). However, at present there is a lack of experimental and theoretical results on this behaviour in a magnetic field or in crossed magnetic and electric fields. The main goal of the present paper is to close this gap. We shall consider a system of a finite number of potential wells separated by barriers. The whole structure is subjected to a magnetic field $\boldsymbol{B}$ parallel to the interfaces or to a crossed magnetic field $\boldsymbol{B}$ and electric field $\boldsymbol{F}$. We believe that the results presented here will give new insight into the surface level behaviour in external fields.

Let us start by considering a system of N rectangular wells of width a separated by $N-1$ barriers of width s and height V_B. Its total width is $\Delta = Na+(N-1)s$. The structure is confined by outer semi-infinite barriers with heights V_L and V_R which, in general, are different. They also may differ from V_B. It is well known that, if $N = 2$, each energy level corresponding to an isolated well as a result of interwell coupling may split into a doublet, if $N = 3$, into a triplet, etc. In this way the band structure of solids is formed. However, because of the presence of outer barriers with heights different from V_B, on increase in N then two of these sublevels start to 'peel off' from the band (in the case of a thin film) or miniband (in the case of an SL). Further we shall assume for simplicity that $V_L = V_R = V_0$. For $V_0 > V_B$ the levels go upwards from the band or miniband and, for $V_0 < V_B$, downwards; their wavefunctions start to localize at the external interfaces. The difference between the two surface states is one of symmetry of the wavefunctions. For instance, for the case $V_0 > V_B$ the antisymmetric surface state lies above the symmetric

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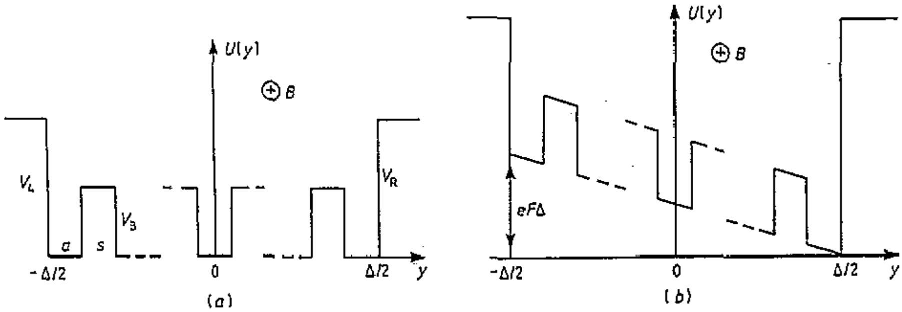

Figure 1. Systems considered: (*a*) finite SL in a uniform magnetic field; (*b*) finite SL in crossed magnetic and electric fields (the latter is assumed to be confined within only the SL). The z axis coincides with the magnetic field direction.

surface state. For rather small N, the interaction between surface levels causes energies of these states to be different but, on increase in N, this difference becomes smaller and smaller and, for large N, one has an almost completely doubly degenerate state.

Let us now apply to the structure a magnetic field of intensity B parallel to the layers (figure 1(*a*)). We choose the gauge where the vector potential $\boldsymbol{A}$ takes the form $\boldsymbol{A} = (-By, 0, 0)$. Then the solution of the Schrödinger equation in the jth well $(1 \leqslant j \leqslant N)$ is

$$\chi_j^{(\mathrm{W})}(y) = A_j^{(\mathrm{W})} U(c^{(\mathrm{W})}, \zeta^{(\mathrm{W})}) + B_j^{(\mathrm{W})} V(c^{(\mathrm{W})}, \zeta^{(\mathrm{W})}) \tag{1a}$$

and in the jth barrier $(1 \leqslant j \leqslant N-1)$

$$\chi_j^{(\mathrm{B})}(y) = A_j^{(\mathrm{B})} U(c^{(\mathrm{B})}, \zeta^{(\mathrm{B})}) + B_j^{(\mathrm{B})} V(c^{(\mathrm{B})}, \zeta^{(\mathrm{B})}) \tag{1b}$$

with

$$c^{(\mathrm{W})} = -(E - p_z^2/2m^{(\mathrm{W})})/\hbar\omega^{(\mathrm{W})} \tag{2a}$$

$$c^{(\mathrm{B})} = -(E - p_z^2/2m^{(\mathrm{B})} - V_{\mathrm{B}})/\hbar\omega^{(\mathrm{B})} \tag{2b}$$

$$\zeta^{(\mathrm{W})} = \zeta^{(\mathrm{B})} = 2^{1/2}(y - y_0)/r_{\mathrm{B}}. \tag{2c}$$

Here $r_{\mathrm{B}} = (\hbar/eB)^{1/2}$, $\omega^{(\mathrm{W})} = eB/m^{(\mathrm{W})}$, $\omega^{(\mathrm{B})} = eB/m^{(\mathrm{B})}$, $y_0 = -p_x/eB$, $m^{(\mathrm{W})}$ and $m^{(\mathrm{B})}$ are the effective masses of electrons in the well and in the barrier, respectively, p_x and p_z are the x and z components of the kinetic momentum $\boldsymbol{p}$, and $U(c, \zeta)$ and $V(c, \zeta)$ are the parabolic cylinder functions [11, 12]. At $y = \pm\infty$ the wavefunction must be finite. Thus, from the properties of parabolic cylinder functions, one has the following solutions: in the region $y > \Delta/2$,

$$\chi_\infty^{(+)}(y) = A_\infty^{(+)} U(c^{(0)}, \zeta^{(\mathrm{B})}) \tag{3a}$$

and in the region $y < -\Delta/2$,

$$\chi_\infty^{(-)}(y) = A_\infty^{(-)} U(c^{(0)}, -\zeta^{(\mathrm{B})}) \tag{3b}$$

$$c^{(0)} = -(E - p_z^2/2m^{(\mathrm{B})} - V_0)/\hbar\omega^{(\mathrm{B})}. \tag{3c}$$

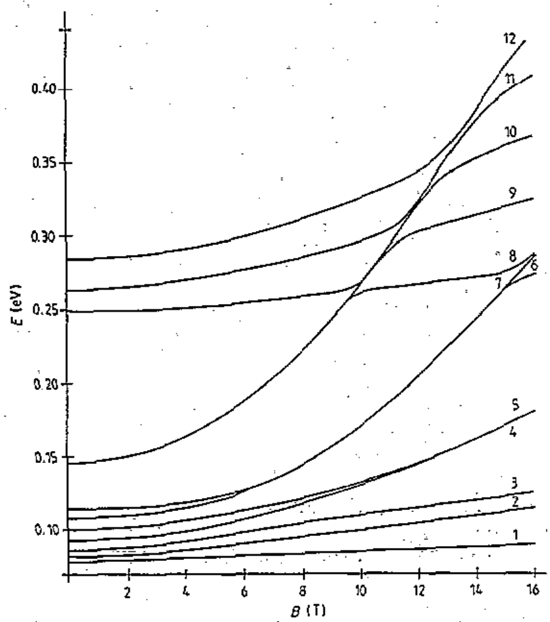

Figure 2. Energies E_i of the levels as a function of B at $F = 0$: 1–7, bulk levels of the first miniband; 8, 9, two surface states of the first miniband; 10–12, bulk levels of the second miniband.

Matching the solutions on each boundary (in the case of the SL, one can choose, similar to [4, 5, 7, 8, 13], Bastard's [14] boundary conditions), we obtain the equation for the determination of the energy levels.

In figure 2 the dependence of the energy on the magnetic field is plotted for the case $N = 9$, $a = s = 4$ nm, $V_0 = 4$ eV, $V_B = 0.2$ eV, $p_x = p_z = 0$, $m^{(W)} = m^{(B)} = 0.067m_e$, with m_e the electron mass. With this choice of p_x and p_z the centre of the magnetic oscillations coincides with the middle of the structure. In the figure, seven levels of the first allowed miniband, two Tamm states of the same miniband and three lowest levels of the second miniband are shown. As we stressed before, Tamm states are almost completely doubly degenerate. This is just the reason why in figure 2 they are not resolved at low magnetic fields. As one can see, the energies of the surface as well as of the bulk levels increase with increasing magnetic field. Tamm state energies increase more rapidly and, when they approach the lowest level of the second miniband, splitting occurs; there is an anticrossing of the lower surface state and bulk level, and the higher Tamm state and the extended level stick together. On further increase in B this paired state approaches the second level of the miniband, and the situation just described is repeated. This is also true for higher states. We have repeated calculations for two more cases: case I, $V_L > V_R = V_B$ (i.e. only one surface state which is localized near the left semi-infinite barrier exists); case II, $V_0 = V_B$ (i.e. all levels in the miniband are extended). They show that both the single Tamm state (case I) and the highest extended level of the first miniband (case II) also anticross with levels of the second miniband on increase in the magnetic field. Case II was studied earlier by Maan [15] who found similar anticrossings in the dependence of the magnetic levels on the cyclotron orbit position y_0 (see figure 9 in [15]). However, in [15] the surface levels are not the subject under consideration.

The bulk levels of the first miniband may also stick together (for higher energies this takes place at weaker fields), and their splitting occurs when they approach a lower surface state. In this case the picture of interaction is similar to that described above. We have performed calculations up to $B = 16$ T. We believe that at stronger fields the levels transform into Landau states, which is a general feature of all quantum-mechanical systems

[16]. However, at such fields the applicability of the effective-mass approximation must be additionally justified [17, 18].

Before considering the combined influence of the electric and magnetic fields, we wish to point out briefly that the electric field F (we assume that it is confined only within the structure considered) applied to the system also lifts the degeneracy of surface states. In this case the wavefunctions take the following forms: in the wells,

$$\chi_j^{(W)}(y) = A_j^{(W)}\mathrm{Ai}[-z_W(y + E/eF - \Delta)] + B_j^{(W)}\mathrm{Bi}[-z_W(y + E/eF - \Delta)] \quad (4a)$$

and, in the barriers,

$$\chi_j^{(B)}(y) = A_j^{(B)}\mathrm{Ai}\{-z_B[y + (E - V_B)/eF - \Delta]\} + B_j^{(B)}\mathrm{Bi}\{-z_B[y + (E - V_B)/eF - \Delta]\} \quad (4b)$$

$z_W = (2m^{(W)}eF/\hbar^2)^{1/3}$, $z_B = (2m^{(B)}eF/\hbar^2)^{1/3}$, and $\mathrm{Ai}(\xi)$ and $\mathrm{Bi}(\xi)$ are Airy functions [11].

The energies of extended states, which undergo Stark localization [19–21], monotonically increase with increasing F. The same behaviour is observed also for higher surface level, but the energy of the lower Tamm state is almost unaffected by the electric field. Whenever the bulk state crosses this surface state, anticrossing occurs. These anticrossings were recently observed experimentally [2] for the case of a single Tamm state.

When both electric and magnetic fields are applied to the structure†, the solutions of the Schrödinger equation are also expressed by (1a) and (1b), but $c^{(W)}$, $c^{(B)}$, $\zeta^{(W)}$ and $\zeta^{(B)}$ are now as follows:

$$c^{(W)} = -[E - p_z^2/2m^{(W)} + \tfrac{1}{2}eF(2y_0 + \gamma^{(W)} - \Delta)]/\hbar\omega^{(W)} \quad (5a)$$

$$c^{(B)} = -[E - p_z^2/2m^{(B)} - V_B + \tfrac{1}{2}eF(2y_0 + \gamma^{(B)} - \Delta)]/\hbar\omega^{(B)} \quad (5b)$$

$$\zeta^{(W)} = 2^{1/2}(y - y_0 - \gamma^{(W)})/r_B \quad (5c)$$

$$\zeta^{(B)} = 2^{1/2}(y - y_0 - \gamma^{(B)})/r_B \quad (5d)$$

$$\gamma^{(W)} = F/B\omega^{(W)} \qquad \gamma^{(B)} = F/B\omega^{(B)}.$$

Figures 3 and 4 characterize the dependence of the energy on the electric field F at fixed B and on the dependence of the energy on the magnetic field B at fixed F, respectively. As one can see from figure 3, the applied in-plane magnetic field leads to a shift in the anticrossings into the region of larger F. At strong magnetic fields, new anticrossings, which are absent at $B = 0$ T, may appear (see figures 3(c) and 3(d)). Very interesting phenomena are observed in the dependence of the energy E on the intensity B at fixed F. As we stressed before, the applied electric field breaks the degeneracy of surface states. The degeneracy of bulk levels, caused by the magnetic field, is also lifted. Energies which at $F = 0$ were almost the same, at $F \neq 0$ have strong anticrossing behaviour. For instance, on increase in B, the higher surface state anticrosses with the lowest level of the second miniband (the location of this anticrossing with increasing F is shifted to smaller B), and a further increase in magnetic field leads to anticrossing between surface states. In turn, the lowest level of the second miniband anticrosses with the higher level, etc. In the first miniband, at large F, new anticrossings, which are absent at $F = 0$, may also appear. Comparison of figures 3 and 4 clearly indicates that characteristic anticrossing behaviour may be achieved in two ways:

† A similar problem for an infinitely deep single potential well was recently solved in [22].

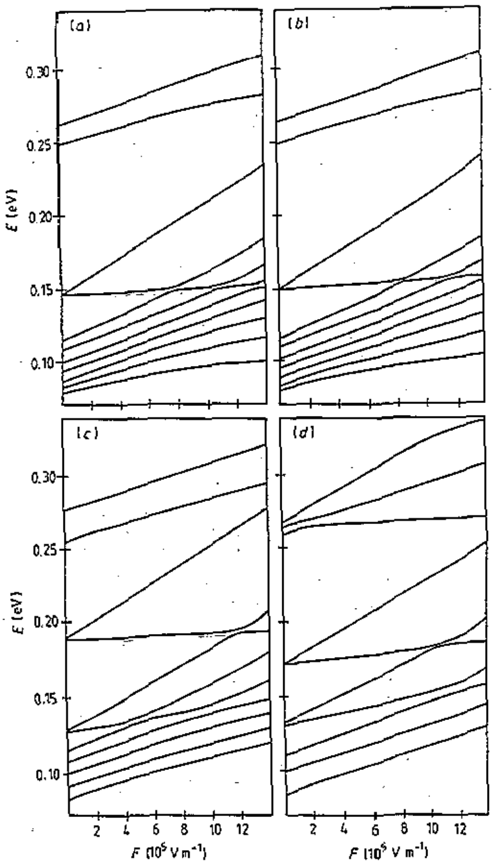

Figure 3. Energies E_i of the levels as a function of F at (*a*) $B = 0$ T, (*b*) $B = 2$ T, (*c*) $B = 6$ T and (*d*) $B = 10$ T.

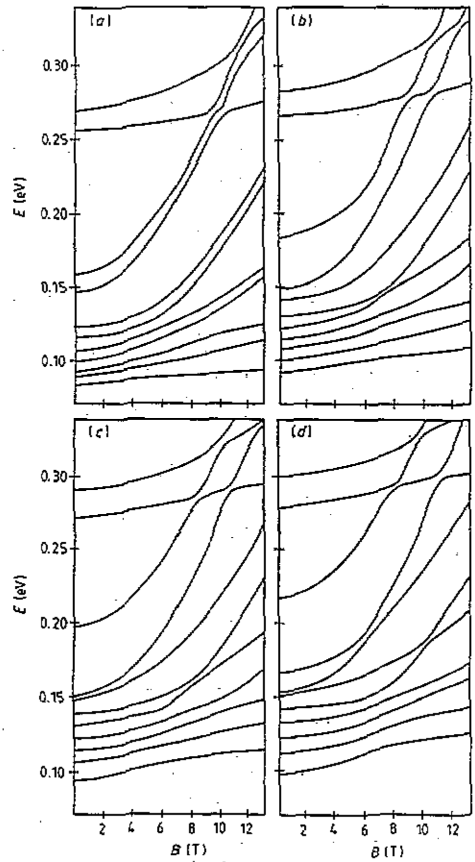

Figure 4. Energies E_i of the levels as a function of B at (*a*) $F = 2 \times 10^5$ V m^{-1}, (*b*) $F = 6 \times 10^5$ V m^{-1}, (*c*) $F = 8 \times 10^5$ V m^{-1} and (*d*) $F = 11 \times 10^5$ V m^{-1}. Comparison with figure 2 shows that the levels, which are degenerate at $F = 0$, strongly anticross when an electric field is superimposed on a magnetic field.

(i) by changing F at fixed $B \geqslant 0$;
(ii) by changing B at fixed $F \neq 0$.

In conclusion, we have investigated, for the first time, the influence of a magnetic field or of crossed magnetic and electric fields on SL surface states. Increasing the magnetic field lifts degeneracy of the surface states and leads to a series of anticrossings between them and the extended states in the first and the second minibands. The most remarkable feature of the influence of crossed fields is also the characteristic anticrossing behaviour of levels as functions of B as well as F. Thus, once again it is confirmed [15, 16, 22] that a continuous transition from electric to magnetic quantization allows one to realize almost arbitrary combinations of interlevel energies which may be used in designing tunable light sources and detectors.

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