Tight-binding model for strongly modulated two-dimensional superlattices

Karel Výborný†‡§ and Ludvík Smrčka†

† Institute of Physics, Academy of Sciences of the Czech Republic, Cukrovarnická 10, 16253 Praha, Czech Republic,

‡ I. Institute of Theoretical Physics, University of Hamburg, Jungiusstr. 9, 20355 Hamburg, Germany

Abstract. Common models describing magnetotransport properties of periodically modulated two–dimensional systems often either directly start from a semiclassical approach or give results well conceivable within the semiclassical framework. Recently, magnetoresistance oscillations have been found on samples with strong unilateral modulation and short period ($d = 15$ nm) which cannot be explained on a semiclassical level (magnetic breakdown [1]). We use a simple fully quantum mechanical model which gives us both magnetoresistance data nicely comparing to the experiments and a good intuitive insight into the effects taking place in the system.

Beginning with the pioneering work of Weiss *et al.*[2] much effort was dedicated to magnetotransport properties of periodically modulated two dimensional systems (2DES). A wide palette of structures has been studied both experimentally and theoretically: with periodic modulation in one direction or in both directions, with modulation by either or both electric and magnetic field, with various modulation strengths and concentrations of electrons (see [3] and references therein). Despite the complexity of many such systems, the experimental data can usually be interpreted within a semiclassical (SC) picture, based on constructing classical trajectories of charge carrier and (if necessary) imposing a quantization condition which reflects the formation of Landau levels in the one–electron spectrum.

In this paper, we refer to a system where the SC prediction contradicts the experimental finding. It is a strongly unilaterally modulated 2DES with modulation period as short as 15 nm (see Section 2 for criterion of short period); it may thus be conceived as an array of weakly coupled quantum wires, see sketch in Fig. 1. Experimentally, these conditions were achieved in a GaAlAs/GaAs superlattice fabricated by cleaved edge overgrowth technique first reported by Deutschmann *et al.* [1], see also more detailed description in [4, 5].

§ To whom correspondence should be addressed (vybornyk@fzu.cz)

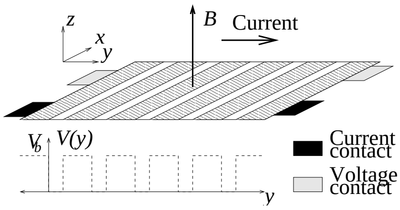

Figure 1. Two–dimensional electron gas with periodic unilateral modulation. Alternatively, the system may be conceived as an array of wires coupled by tunnelling.

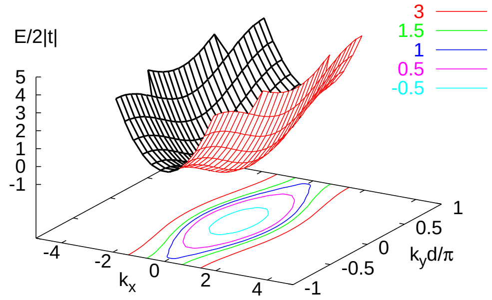

Figure 2. Band structure in zero magnetic field: all modulation bands (in y–direction) except for the lowest are discarded. Fermi contours (related to real space trajectories) are closed for $-2|t| < E_F < 2|t|$ and open for $E_F > 2|t|$.

1. Model for Zero Magnetic Field: Semiclassics

Since the potential in our system is separable, zero magnetic field band structure is an effectively one–dimensional problem. Motion along the wires (x direction) is free and motion across the wires (y direction) can be described by a Kronig–Penney model. For the structure studied in [1], we find that the lowest band of the one–dimensional band structure in the y direction is narrow ($4|t| \approx 3.8$ meV wide), has nearly a cosine form and is well separated from the higher bands (≈ 60 meV). Regarding the experimentally accessible concentrations of electrons the Fermi level E_F lies always well below the second band (that means naturally also deep below V_b, the potential of barriers in the superlattice) and thus, from now on, we will discard all but the lowest modulation band. Note that this considerable simplification is rendered by the shortness of the modulation period (which introduces large modulation band gaps). The zero field band structure is therefore (see Fig. 2)

$$E(k_x, k_y) = \frac{\hbar^2 k_x^2}{2m} - 2|t| \cos k_y d \,. \qquad (1)$$

Let us now examine the SC model of a system with such a band structure. The real space trajectory of an electron subject to a perpendicular magnetic field B will be the Fermi contour $E_F = E(k_x, k_y)$ scaled by $\ell^2 = \hbar/eB$ and rotated by $90°$. Evidently, this is a closed trajectory for $-2|t| < E_F < 2|t|$ (resembling circular orbits of electrons moving in a plane, i.e. 2D–like behaviour) and an open trajectory for $E > 2|t|$ (corresponding to motion along the wires, i.e. 1D–like behaviour). Shubnikov–de Haas oscillations of the magnetoresistance are predicted for the former case (through the SC quantization condition: real space trajectory must enclose integer multiple of magnetic flux quanta $\Phi_0 = h/e$, [6]). In contrast, the magnetoresistance is expected to be non-oscillatory in the latter case (there is no quantization condition for open trajectories).

This model, however, does not always agree with the experiments [1]: $1/B$–periodic oscillations were observed even for $E_F > 2|t|$ (see Fig. 5) being referred to as magnetic breakdown. Since the type of periodicity is the same as for $-2|t| < E_F < 2|t|$ we can extend the SC model and claim that electrons tunnel between the open trajectories and, thus, form loops for which the usual quantization condition is to be fulfilled. This is however an assumption strange to classical theories and we may ask how many such *ad hoc* assumptions we need in order to reconcile theory and experiment while pretending that electrons in such systems always obey classical and not quantum mechanical laws.

As it was mentioned above this situation occurs owing to the strong modulation (i.e. width of the lowest modulation band is as low as the Fermi level, $E_F \approx 4|t|$) and the shortness of the modulation period ($d^2 \lesssim 3h^2/(2|t|m)$).

2. Quantum Mechanical Model

The system is described by the Hamiltonian

$$H = \frac{1}{2m}(p_x + eBy)^2 + \frac{1}{2m}p_y^2 + V(y) \tag{2}$$

in the Landau gauge $\vec{A} = (By, 0, 0)$ (we set $e = |e|$). The restriction to the lowest modulation band is equivalent to the tight–binding ansatz (used also by Wulf *et al.* [7])

$$\Psi(x, y) = \frac{1}{\sqrt{2\pi}}\exp(ikx)\psi_{k,n}(y) = \frac{1}{\sqrt{2\pi}}\exp(ikx)\sum_j a_j(k)\varphi(y - jd)\,,$$

$$\langle\varphi_i|H_y|\varphi_j\rangle = -|t|\delta_{i,j\pm 1}$$

where $\varphi(y - jd)$ or $|\varphi_j\rangle$ denotes the ground state (more precisely Wannier state) in the j-th well of the modulation potential and n is Landau band index. Moreover, we assume that t does not change with magnetic field. This is plausible unless the magnetic field is extremely strong ($\ell^2 k_F \ll d$, k_F is the Fermi wavevector; in such a case a 2DES is formed inside one quantum wire).

The Hamiltonian can be now written as a matrix

$$H_{jl}(k) = |t|\left[\alpha^2((k/K) + j)^2\delta_{j,l} - \delta_{j,l\pm 1}\right]\,, \tag{3}$$

$$\alpha^2 = \frac{e^2B^2}{m}\cdot\frac{d^2}{2|t|} = \left(\frac{\hbar\omega_{\text{eff}}}{2|t|}\right)^2, \qquad K = d\frac{eB}{\hbar}$$

which depends (up to the scaling of k and energy) on a single dimensionless parameter α.

If the system is infinite in the y direction, the spectrum is K–periodic in k (due to invariance to magnetic translations) and its spectrum coincides with the one of a *fictitious* 1D particle in a periodic cosine potential (Mathieu equation) [8]

$$-\frac{\hbar^2}{2m}\chi''(\xi) - \chi(\xi)2|t|\cos K\xi = E\chi(\xi)\,. \tag{4}$$

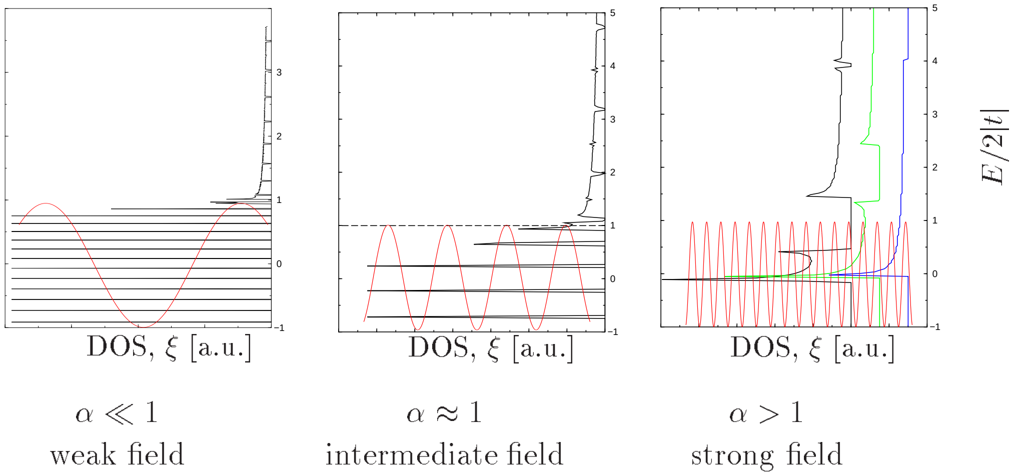

Figure 3. Density of states at different magnetic fields and corresponding potential for the fictitious particle. At low magnetic field ($\alpha \ll 1$) there are almost sharp Landau levels for $-2|t| < E < 2|t|$ and an almost 1D–like DOS ($\propto 1/\sqrt{E}$) for $E > 2|t|$: this corresponds to the semiclassical model. At higher magnetic fields ($\alpha \approx 1$) the Landau levels broaden into Landau bands (an effect of the modulation) and gaps in the 1D–like region become more pronounced. Finally for $\alpha > 1$ there remains only one broad Landau band in the $-2|t| < E < 2|t|$ region and the gaps still grow (for our system parameters the DOS displayed in the graph on the right correspond left to right to $B = 5$, 7 and 11 Tesla).

Note, that the cosine potential changes with magnetic field (via K). This allows for an easy notion of what the spectrum looks like for different values of α (see Fig. 3). For instance, if the period of the cosine potential is large (it means small K, more precisely $\alpha \ll 1$), each of the periods contains a broad potential well: near the bottom it may be approximated by a quadratic potential and we thus obtain almost equidistantly spaced levels. Since these cosine wells are only weakly coupled to each other (barriers between them are thick), the band structure will comprise of narrow bands (Fig 3 left). On contrary, states with an energy $E > 2|t|$ high above the top of the cosine potential (but still under the second modulation band, i.e. deep under V_b, see Fig. 1) will percept this potential only as a perturbation: the spectrum will be almost as of a free 1D particle (parabolic) and with small gaps opening at $k = \pm\frac{1}{2}K$ due to the underlying potential perturbation.

Plotting the density of states (DOS) at the Fermi level as a function of magnetic field we can see that our model reproduces very precisely the magnetoresistance oscillations for various electron concentrations (Fig. 4).

3. Transport calculations

Based on the Kubo formula (linear response to applied bias) we computed the conductivity tensor components (see [3]) at zero temperature (for brevity we write E

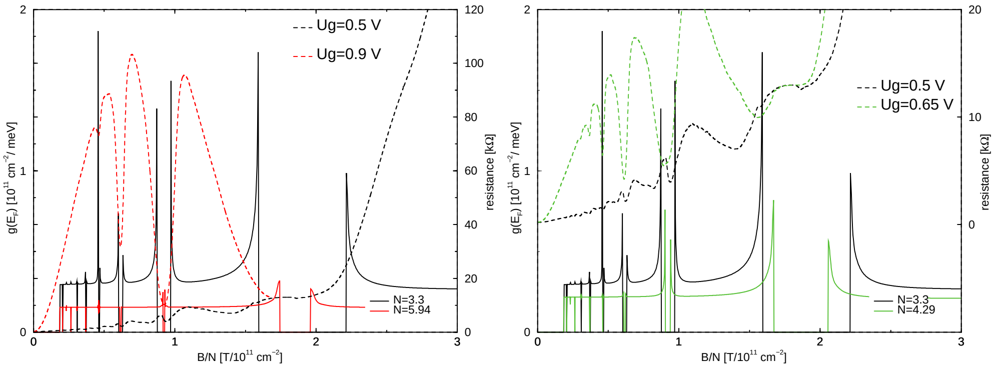

Figure 4. Density of states (solid lines) compared to the experimental magnetoresistance (dashed lines; reprinted with kind permission of R. A. Deutschmann): gaps in the DOS agree with the extrema of the magnetoresistance. Gate voltages are given for the experimental curves and corresponding 2D electron concentrations in 10^{-11} cm^{-2} are given for the DOS. All the displayed curves correspond to $E_F > 2|t|$.

for the Fermi level)

$$\begin{aligned}
\sigma_{xx}(E) &= \frac{2}{\pi\Gamma d} \cdot \frac{e^2}{h} \cdot \frac{\mathrm{sgn}(g(E))}{g(E)} + \\
&\quad + \frac{4\pi\Gamma}{d} \cdot (\hbar\omega)^2 \cdot \frac{e^2}{h} \cdot g(E) \sum_{n' \neq n} \left(\frac{\langle \psi(k,n')|\hat{y}|\psi(k,n)\rangle}{E(k,n') - E(k,n)} \right)^2 \\
\sigma_{yy}(E) &= \frac{4\pi\Gamma}{d} \cdot \frac{e^2}{h} g(E) \sum_{n' \neq n} \Big(\langle \psi(k,n')|\hat{y}|\psi(k,n)\rangle \Big)^2 \\
\sigma_{xy}(E) &= e\frac{\partial N(E)}{\partial B} + \frac{4\pi\hbar\omega}{d} \cdot \frac{e^2}{h} g(E) \sum_{n' \neq n} \left(\langle \psi(k,n)|\hat{y}|\psi(k,n')\rangle \right)^2 ,
\end{aligned}$$

including the factor two for spin. Here $\omega = eB/m$, $N(E)$ is number of states with energy less than E, $\hat{y}$ is the y–coordinate operator and $\mathrm{sgn}(g(E))/g(E)$ is to be understood as 'zero for $g(E) = 0$ and $1/g(E)$ else'. We treated the impurity scattering within the c–number approximation for self–energy (Γ denotes its imaginary part); Γ has then the meaning of an inverse relaxation time, $\Gamma = \hbar/\tau$.

The first term of the xx–component of conductivity can be attributed to electrons moving along open orbits. If the wires in the superlattice were decoupled, the DOS would be the same as of a 1D electron gas ($g(E) \propto 1/\sqrt{E}$) and the first term in σ_{xx} would be simply proportional to $\sqrt{E}$, i.e. the electron velocity. This term is proportional to the relaxation time (as may be expected). In contrast, σ_{yy} (as well as the second term of σ_{xx}) is inversely proportional to the relaxation time: this means that conduction across the wires is due to *inter*–Landau–band scattering (sumation over $n' \neq n$) introduced by impurities.

The first term in σ_{xy} introduces Hall plateaus of quantized conductivity when E lies in a gap; it vanishes in the classical limit. The second term does not depend on

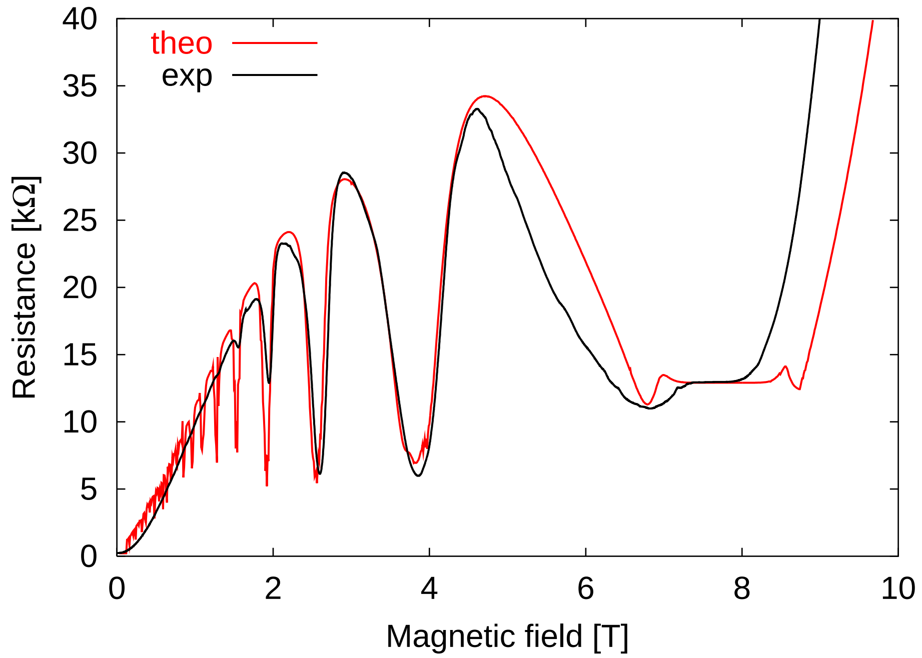

Figure 5. Theory prediction and experimental magnetoresistance (reprinted with kind permission of R. A. Deutschmann). According to the semiclassical theory there should be no oscillations ($E_F > 2|t|$). For the imaginary part of the self–energy (inverse relaxation time) the phenomenological ansatz $\Gamma(E, B) \propto \sqrt{B}$ was used (according to [9]).

the relaxation time. It is proportional to B (appearing in ω) and resembles thus the classical Hall conductivity.

To be able to discuss the experimental data we have to address the relation between the computed conductivity components and measured resistance at last. Due to technological reasons resistivity components ϱ_{yy} and ϱ_{xy} could not be measured separately. We expect that the measured resistance is a mixture of these two quantities, $c\varrho_{yy} + \varrho_{xy}$ and this allows us to fit the experimental curves quite well with a single fitting parameter (Fig. 5) for Fermi energies $E_F > 2|t|$. The agreement is worse but still at least qualitative for $E_F \approx 2|t|$.

4. Conclusion

We investigated a two–dimensional electron system for which the usual semiclassical approach fails to predict correct magnetoresistance behaviour. The wide gap between the lowest and second lowest modulation band was the crucial prerequisite for this to happen which in turn depends on the unusually short period of the modulation potential. The observed $1/B$–periodic magnetoresistance oscillations may be understood as a consequence of electron tunnelling between semiclassical orbits. We presented a simple quantum mechanical model based on a tight binding approximation which can account very well for these oscillations. Very simplistic transport calculations are in nearly quantitative agreement with the experiment for a wide range of electron concentrations. Outside this range qualitative agreement is still retained.

One of the authors (KV) would like to acknowledge discussions with Daniela Pfannkuche and Alexander Chudnovskiy. This work has been partly supported by the Grant Agency of the Czech Republic under Grants No. 202/01/0754 and No. 202/03/0431.

5. References

[1] R. A. Deutschmann *et al.*, Physica E **6**, 561 (2000).
[2] D. Weiss, K. von Klitzing, K. Ploog, and G. Weinmann, Europhys. Lett. **8**, 179 (1989).
[3] K. Výborný, L. Smrčka, and R. A. Deutschmann, cond-mat/0206212 .
[4] R. A. Deutschmann *et al.*, Phys. Rev. Lett. **86**, 1857 (2001).
[5] R. A. Deutschmann, *Two dimensional electron systems in atomically precise periodic potentials, Selected topics of Semiconductor Physics and Technology, Vol. 42* (University of Technology Munich, Munich, 2001), PhD. thesis, ISBN 3-932749-42-1.
[6] N. Ashcroft and N. Mermin, *Solid State Physics* (Saunders College Publishing, Orlando, 1976), p. 232.
[7] U. Wulf, J. Kučera, and A. MacDonald, Phys. Rev. B. **47**, 1675 (1992).
[8] To see the equivalence between Eq. 3 and Eq. 4, substitute $\chi(\xi) = e^{ik\xi}\sum_n a_n e^{inK\xi}$ into Eq. 4 in accordance with Bloch's theorem. Then $H_{jl}(k)$ turns out to be the matrix of the Hamiltonian in Eq. 4 in the basis $e^{ik\xi}e^{inK\xi}$, $n = 0, \pm 1, \pm 2, \ldots$.
[9] A. Manolescu *et al.*, Surf. Sci. **361/362**, 513 (1996).