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LETTER TO THE EDITOR

Landau levels in confined two-dimensional electron gas: calculation by the finite-element method

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Abstract. The finite-element method for electronic structure calculations for narrow two-dimensional systems in perpendicular magnetic fields is suggested as a feasible alternative to the conventional tight-binding model. The accuracy and versatility of the method are illustrated for the case with a rectangular well. As an example of a more realistic problem, the influence of the magnetic field on the charge-density distribution in a narrow two-dimensional sample with an oblong well at its centre is investigated.

Narrow two-dimensional electron systems with electrons spatially confined in a controlled way are pertinent to the most significant recent developments in semiconductor physics. The high speeds and novel electronic properties of these structures make them promising candidates for a new generation of electronic devices. Therefore, it is worth making efforts to clarify and describe the phenomena that occur in such systems.

In many cases, fundamental electronic properties of the narrow systems follow from simple analytically solvable models. Nevertheless, for a more realistic description numerical calculations are often required. The lattice tight-binding model has been most frequently used to determine the electronic structure in both the zero and a strong magnetic field perpendicular to a two-dimensional system (Harper 1955, Rabinovitch 1969, Schweitzer *et al* 1985, Lovesey 1988, Czycholl and Ponischowski 1988, Kramer and Mašek 1988). Recently, this model has been carefully reinvestigated in comparison with the continuum free-electron model (Gudmundsson *et al* 1988).

In this contribution, we suggest the finite-element method as a feasible alternative to the conventional tight-binding model for treating narrow two-dimensional electron systems. The potential of this method was first recognised by engineers. Subsequently, as its mathematical foundations became established, it was applied with success to a great variety of fields including quantum mechanics (*Computer Physics Reports* 1987). Here, we attempt to utilise it for the first time in calculating the electronic structure of a confined two-dimensional electron gas. For application to one-dimensional electron systems in magnetic fields see, e.g., Maan (1987).

We assume a two-dimensional system of non-interacting electrons in the magnetic field $\boldsymbol{B} = (0, 0, B)$ oriented perpendicularly to the system. The length and the width of

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the system are denoted by L_x and L_y, respectively. The wavefunction $\psi(x, y)$ of an electron satisfies the periodic boundary conditions in the x direction

$$\psi(-L_x/2, y) = \psi(L_x/2, y) \qquad y \in \langle -L_y/2, L_y/2\rangle \tag{1}$$

and the Dirichlet boundary condition in the y direction

$$\psi(x, -L_y/2) = \psi(x, L_y/2) = 0 \qquad x \in \langle -L_x/2, L_x/2\rangle. \tag{2}$$

For simplicity, the spin is not taken into account. The electron motion is described by the one-electron Hamiltonian with the potential $V(x, y)$

$$H = (1/2m)(p_x + eBy)^2 + (1/2m)p_y^2 + V(x, y) \tag{3}$$

where e is the charge on an electron and m is its mass.

The basic idea in using the finite-element method for our problem is to cover the region $\langle -L_x/2, L_x/2\rangle \times \langle -L_y/2, L_y/2\rangle$ by a mesh of knots and to express the wavefunction as a linear combination of the basis functions localised around the knots, i.e. each basis function is non-zero only in a finite region surrounding a knot (the mathematically correct definition can be found, e.g., in Prenter 1975). This is reminiscent of the tight-binding method in which the Wannier functions localised around the equidistant positions of atoms form a basis set. Usually, the Wannier functions themselves are not specified but are introduced into the problem only through the matrix elements of the zero-field Hamiltonian. The effect of the magnetic field is subsequently incorporated into the tight-binding Hamiltonian via the Peierls substitution (Peierls 1933, Luttinger 1951, Hofstadter 1976, Wannier 1978). In the finite-element method the basis functions are given explicitly in an analytic form. This allows the direct evaluation of all matrix elements, and the resulting eigenfunctions are also given analytically for the whole region $\langle -L_x/2, L_x/2\rangle \times \langle -L_y/2, L_y/2\rangle$—similarly to the eigenfunctions of the continuum free-electron model. In the conventional tight-binding method the presence of a periodic potential is assumed implicitly and the zero-field energy spectrum is given by a bounded Bloch band. The present approach represents only a convenient way of transcribing the differential equation into a difference one; the choice of knots is not related to the actual crystal structure and the zero-field solution corresponds rather to the free-electron spectrum than to the Bloch band.

To illustrate the method, we first consider the simplest case—equation (3) with $V = 0$. This choice allows the separation of variables in the eigenfunctions of H and the reduction of the problem to one dimension. The eigenfunctions can be written in the form

$$\psi(x, y) = e^{ikx} u_{nk}(y). \tag{4}$$

The functions $u_{nk}(y)$ are the solutions to the equation

$$-(h^2/2m)\, d^2/dy^2 + (m\omega_c^2/2)(y - Y)^2 u_{nk}(y) = E_{nk} u_{nk}(y) \tag{5}$$

where $\omega_c = |e|B/m$ and the coordinate Y is related to the wavevector $\boldsymbol{k}$ by the expression $Y = l^2 k$, $l^2 = h/m\omega_c$.

The equidistant mesh of $N+1$ knots $y_i = -L_y/2 + ia$, $a = L_y/N$, $i = 0, 1, \ldots, N$, divides the interval $\langle -L_y/2, L_y/2\rangle$ into finite elements and the basis functions are localised around the knots y_i, $i = 1, \ldots, N-1$. The simplest version of the method is based on the piecewise-linear basis functions $F_i \in C^0$. The function F_i, $i = 1, \ldots, N-1$, differ from zero only for $y_{i-1} < y < y_{i+1}$ and are determined by the conditions $F_i = 1$, $F_{i-1} = F_{i+1} = 0$. More precise approximations use cubic splines $B_i \in C^2$. Each B_i is non-zero

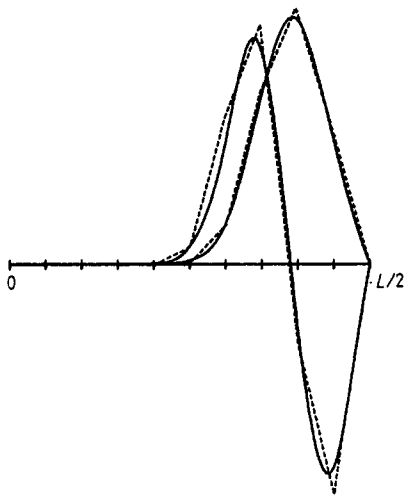

Figure 1. The first two eigenfunctions in a narrow channel of width $L = 10^{-7}$ m (only its right-hand half is sketched), calculated by the finite-element method using linear (broken curve) and cubic (full curve) splines. The magnetic field $B = 5$ T, the wavevector $k = 3 \times 10^{-8}$ m^{-1}, the number of knots = 21.

only between y_{i-2} and y_{i+2} and in these two knots the value of B_i, its first derivative and its second derivative are equal to zero. The cases $i = 0, 1, N-1, N$ need special treatment. The explicit form of F_i, as well as that of B_i, may be found, e.g., in Prenter (1975).

The matrix form of equation (5) is obtained via a direct evaluation of the matrix elements of H between the functions F_i or B_i. Using the set of piecewise-linear functions we arrive at the tridiagonal Hamiltonian and overlap matrices. The error of the method in this case is proportional to a^2. Cubic functions B_i lead to seven-banded matrices. The increase in complexity in the preparatory part, i.e. in the evaluation of the matrix elements, and in the numerical treatment of the matrix problem, is compensated for by the higher precision of calculation: the error is proportional to a^4. Consequently the number of spline functions included and the dimensions of the matrices may be reduced. This appears to be advantageous particularly in two-dimensional problems.

In the zero-magnetic-field case the problem is reduced to the one-dimensional, infinitely deep potential well. Then the analytic solutions are known and can be directly compared with the results obtained by the finite-element method. Both the linear and the cubic splines stand this test very well. Even for the quite small number of finite elements, $N = 10$, the method fits the analytic solution with an accuracy better than (at least for the first three eigenenergies) 10^{-3} and 10^{-6} for eigenfunctions (with respect to the norm) and 5×10^{-2} and 3×10^{-5} for eigenvalues when the linear and cubic splines are used, respectively.

In strong magnetic fields, the wavefunctions are localised around the centre of motion Y and the differences between the linear and cubic splines become more pronounced. Naturally, the linear spline cannot follow a smooth curve of an eigenfunction if the distance between the knots is comparable with the distance between two neighbouring eigenfunction nodes. The conditions are not so stringent for the more accurate smooth cubic splines, as illustrated in figure 1. Moreover, the numerical convergence test for eigenvalues performed for the linear and cubic splines confirms that the approximate eigenvalues are higher than the exact values and that the error decreases as $1/N^2$ for linear splines and as $1/N^4$ for cubic splines, as follows from the error analysis. Figure 2 shows examples of the wavefunctions and the current distributions calculated by the

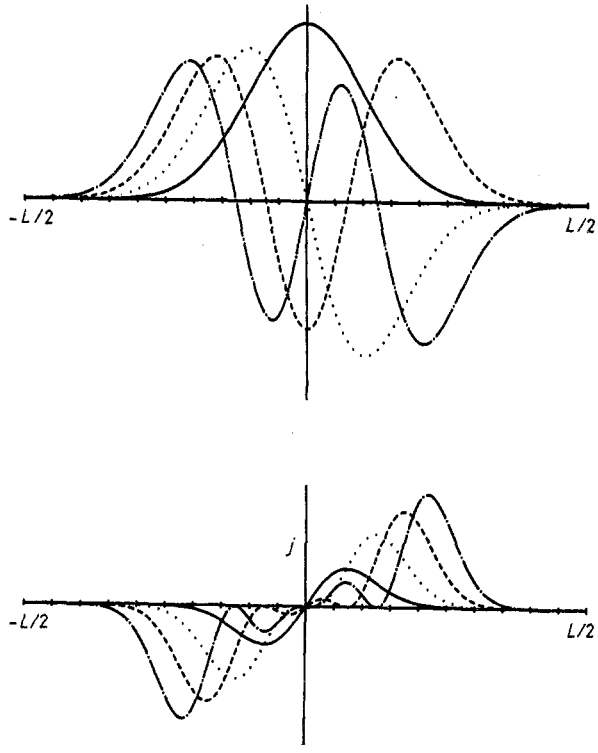

Figure 2. The first four eigenfunctions (upper graph) and the corresponding current distributions (lower graph) calculated by the finite-element method using cubic splines for an infinite rectangular channel of width $L = 2 \times 10^{-7}$ m, placed in a perpendicular magnetic field $B = 0.3$ T. The wavevector $k = 0$. The number of knots = 21.

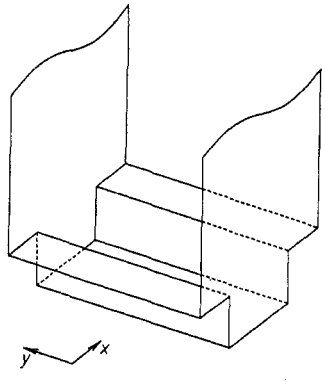

Figure 3. Sketch of the potential in the two-dimensional system with an oblong well at its centre. The system length and width are 3×10^{-8} m; the length, width and depth of the well are 1.4×10^{-8} m; 3×10^{-8} m and 1.25×10^{-22} J; respectively.

finite-element method for an infinite rectangular channel placed in a perpendicular magnetic field.

Let us now consider a more realistic model with a non-zero potential $V(x, y)$. In order to show the versatility of the present method, let us investigate a narrow two-dimensional system with an oblong well at its centre as an example of a true two-dimensional problem (figure 3). This problem can simply be treated by constructing a

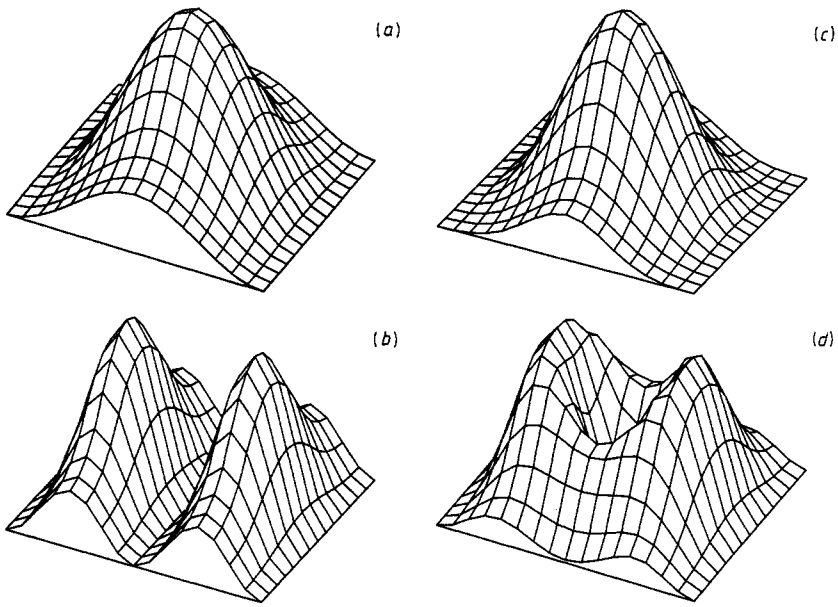

Figure 4. The charge-density distribution in the system outlined in figure 3, calculated by the finite-element method using bilinear splines. (*a*) and (*b*) correspond to the system without magnetic field, (*c*) and (*d*) to the system with the magnetic field $B = 10\,\mathrm{T}$. The charge densities for the first two eigenenergies are depicted in (*a*), (*c*) and (*b*), (*d*), respectively. The eigenenergies $E_1(0) = 1.15 \times 10^{-22}\,\mathrm{J}$, $E_2(0) = 2.94 \times 10^{-22}\,\mathrm{J}$, $E_1(B) = 1.45 \times 10^{-22}\,\mathrm{J}$ and $E_2(B) = 2.80 \times 10^{-22}\,\mathrm{J}$ are comparable with the well depth.

rectangular grid and bilinear or bicubic splines. More details about the construction of various grids and two-dimensional splines can be found in Prenter (1975). Figure 4 shows the distribution of the charge density $\psi^*\psi$ in the system sketched in figure 3, where the wavefunction ψ satisfies the boundary conditions (1) and (2).

Let us investigate the influence of the magnetic field on the eigenenergies and the corresponding eigenfunctions. For the lowest energy the influence of the magnetic field on the charge-density distribution causes only small changes in the shape of the distribution (see figures 4(*a*), (*c*)), indicating that the wavefunction is localised in the well more strongly in the magnetic field. In contrast, the distribution for the second eigenenergy changes very dramatically (see figures 4(*b*), (*d*)). It appears that the wavefunction is again localised strongly in the well, but is now shifted towards the edges of the well, so that a deep depression appears at the centre. The magnetic field enables the electrons to move also across the channel. Figure 4(*d*) documents the fact that the electron motion occurs predominantly along the well edges.

In conclusion, the possibility of making use of the formal simplicity and versatility of the finite-element method for solving bound-state problems in narrow two-dimensional systems in magnetic fields has been outlined. Note that even the present preliminary results demonstrate that the finite-element method can be successfully used for calculations of the electronic structure of a two-dimensional electron gas in a magnetic field with moderate effort, and that this method can serve as an alternative for the conventional tight-binding model. A more detailed discussion of problems connected with actual calculations as well as practical applications of the method to scattering will be published.

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