UNITED NATIONS EDUCATIONAL, SCIENTIFIC AND CULTURAL ORGANIZATION
INTERNATIONAL ATOMIC ENERGY AGENCY
INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS
I.C.T.P., P.O. BOX 586, 34100 TRIESTE, ITALY, CABLE: CENTRATOM TRIESTE

SMR.998d - 15

Research Workshop on Condensed Matter Physics
30 June - 22 August 1997
MINIWORKSHOP ON
QUANTUM WELLS, DOTS, WIRES
AND SELF-ORGANIZING NANOSTRUCTURES
11 - 22 AUGUST 1997

"Electron States in Periodic Nanostructures Subjected to a Strong Magnetic Field"

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ELECTRON STATES IN PERIODIC NANOSTRUCTURES SUBJECTED TO A STRONG MAGNETIC FIELD

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to be published: **Proceedings of 7th International Conference on Megagauss Magnetic Field Generation and Related Topics ("MEGAGAUSS - VII"): "Megagauss and Megaampere Technology and its Applications", Sarov, VNIIEF, 1997.**

1. Introduction

The quantum mechanical problem of Bloch electron in an external magnetic field attracts more and more attention of physicists. The basic ideas about the nature of a Bloch electron spectrum were laid down by Zilberman [1], Zak [2], Azbel [3], Rauh [4], Wannier [5] and Hofstadter [6]. Significant progress has been recently made in the analysis of the nature of electron energy spectrum, wave functions and symmetry of electronic states. At the present time the analytical and numerical methods of calculations of an electronic states have also been developed.

A brief mention should be made of the basic results obtained in the tight-binding and nearly-free-electron approximations. Let $E(\mathbf{k})$ in the tight-binding approximation describe the electron energy as a function of the quasimomentum $\mathbf{k}$. The simplest way to acount for the influence of a magnetic field on a Bloch electron is the Peierls substitution. It deals with the replacement of $\hbar\mathbf{k}$ in $E(\mathbf{k})$ by $E(-i\hbar\nabla - e\mathbf{A}/c)$, where $\hbar$ is the Planck's constant, e is the electron charge, c is the light velocity, $\mathbf{A}(\mathbf{r})$ is a vector-potential. Then the Schrödinger equation to be solved is

$$E\left(-i\hbar\nabla - \frac{e}{c}\mathbf{A}(\mathbf{r})\right)\psi = E\psi. \tag{1}$$

If the energy $E(\mathbf{k})$ in 2D-band is choosen as

$$E(\mathbf{k}) = 2E_0(\cos k_x a + \cos k_y a) \tag{2}$$

and the Landau gauge has the form $\mathbf{A}(0, Hx, 0)$ (a is a lattice constant) then the quasimomentum component k_y becomes a constant of motion. Therefore, the solution of Eq.(1) can be written in the form $\psi(x,y) = \exp(ik_y y)U(x)$. It leads to a discrete Schrödinger equation in a quasiperiodic potential (Harper's equation) [6]

$$U(x+a) + U(x-a) + 2\cos\left(\frac{eHa}{c\hbar}x - k_y a\right)U(x) = \varepsilon U(x), \tag{3}$$

where $\varepsilon = E/2E_0$. By shifting the zero point of x, Eq.(3) can be transformed to the following one

$$C_{n+1} + C_{n-1} + 2\cos(2\pi n\, p/q - \nu)C_n = \varepsilon C_n. \tag{4}$$

In the difference equation (4) C_n is the value of the function $U(x)$ on the nth site, $p/q = a^2/2\pi l_H^2$ gives the number of flux quanta threading a unit cell area a^2. Here $l_H = \sqrt{c\hbar/eH}$ is the magnetic length. The matrix equation (4) is called as Harper's equation. Harper's equation has a simple form but the structure of spectrum ε is quite complicated. When the number of flux quanta per unit cell p/q is a rational number, Eq.(4) is periodic on n with period q. It means that every energy band (2) splits into q subbands, and the energy becomes a function of k_y. In the opposite case, when the ratio of p/q is an irrational number, the quantity of subbands is infinitely large. This fact was predicted by Azbel [3] who proved that the

energy spectrum has the form of Cantor set when p/q is irrational. Hofstadter solved Eq.(4) numerically and obtained the spectrum (see fig.1) which was called as "a butterfly". The tight-binding approximation was also discussed in [8, 9, 10].

The well-known alternate approach to treating the problem (the nearly-free-electron approximation in the Landau basis) has been discussed in [1, 4, 8, 9]. The Landau functions satisfying the generalized Bloch conditions are choosen as non-perturbated functions. It means that under the translation on vector $\mathbf{a}_n = n_1\mathbf{a}_1 + n_2 q\mathbf{a}_2$ (n_1 and n_2 are integer numbers, $\mathbf{a}_1$ and $\mathbf{a}_2$ are the vectors of a unit cell), the electron quantum state is characterized by the same value of quasimomentum $\mathbf{k}$. If the magnetic field satisfies the condition $\mathbf{h}[\mathbf{a}_1, \mathbf{a}_2] = 4\pi p/q$, where $\mathbf{h} = |e|\mathrm{H}/\hbar c$, then under the action of the magnetic translation operator the wave function transforms as

$$\hat{T}_{\mathbf{a}}\psi(\mathbf{r}) = \psi(\mathbf{r} + \mathbf{a})\exp\left(i\mathbf{r}[\mathbf{h}, \mathbf{a}]/2\right) = \exp(i\mathbf{k}\mathbf{a})\psi(\mathbf{r}).$$

When the weak periodic perturbation $V(x,y) = 2V_0\left(\cos[2\pi x/a] + \cos[2\pi y/a]\right)$ is introduced the Schrödinger equation for the coefficients of expansion of the wave function in terms of Landau states C_n has the form [11]

$$\exp(-iqak_x a/p)C_{n+1} + \exp(iqak_x a/p)C_{n-1} + 2\cos(qak_y/p + 2\pi nq/p)C_n = \varepsilon C_n. \qquad (5)$$

Eq.(5) describes the structure of electron states formed from the single Landau level. Eq.(5) is similar to Harper's equation (3) , however, it is periodic in n with the period p, but not q. The later means that each Landau level splits under the action of the periodic potential into p subbands and the energy depends upon k_x and k_y. The full width of the band formed at the position of the Landau level equals

$$\Delta E_N = 8V_0 L_N^0\left(\frac{2\pi^2 l_H^2}{a^2}\right)\exp\left(-\frac{\pi^2 l_H^2}{a^2}\right), \qquad (6)$$

where $L_N^0(x)$ is a Laguerre polynomial. The energy ε in (5) is measured in units of ΔE_N (see Eq.(6)).

The important stage in the development of a knowledge about the nature of electron states in a periodic potential and in a uniform magnetic field was created by Kohmoto et al. [10]. The total energy of 2D-electrons was calculated for the square, triangular and hexagonal lattices. They also computed the Fermi energy as a function of number of magnetic flux quanta threading a unit cell for a fixed electron density. It is shown that the total energy has a cusp (local minimum) at the position where the Fermi energy jumps across a gap. The minimum of a total energy occurs when the number of flux quanta per electron is equal to unity.

A mention should be made of interesting papers by Zilberbauer et al. [12,13] where the solution of Schrödinger equation is decomposed not upon Landau functions, but on the functions calculated in the symmetric gauge of the vector-potential $\mathrm{A}(-Hy/2, Hx/2, 0)$. This solution is invariant with respect to magnetic translations. Such functions were originally discovered by Ferrari [14]. The results of calculating electron spectra for arrays of quantum dots and antidots in a magnetic field are displayed in [12] under the following parameters of the lattice: a=500 nm, V_0=5 meV. The 2D-potential shape in [12] is designed by different periodic functions allowing Fourier series decomposition.

This is an established fact that in the classical limit a system of antidots in a magnetic field exhibits the phenomenon of dynamical chaos, that in the quantum limit this one is embodied in the structure of electron energy spectrum. It is found in [13] that the nearest-neighbour level distribution in this problem changes with respect to magnetic field from Poissonian to GUE for different points of the Brillouin zone.

The experimental study of electron phenomena in periodic and magnetic fields is not as successful as the theoretical one in spite of the fact that this problem is very attractive. In order to observe the effects dealing with the rebuilding of Landau spectrum it is necessary to apply a very strong magnetic fields. Actually, the magnetic length $l_H = 26/H^{1/2}$ nm (H is measured in Tesla) and in the fields about 10 MGs the number of magnetic flux quanta passing through a unit cell with the ordinary lattice constant a=0.3 nm has the order of 10^{-1}. It is easy to see in fig.1 (see also Eq.(6)) that at such values of flux p/q the spectrum consists of the single Landau levels.

In recent years the essential progress in the creation of 2D-lattices consisting of quantum dot and antidot arrays has been achived [15,16]. Such structures can be obtained in a process of the epitaxial growth due to the self-organization. An equilibrium shape of a 2D-lattice arised from single islands is determined by a relation between surface energy, elastic energy and other parameters. In particular, two-dimensional lattices with periods 15-30 nm formed by quantum dots of $(In,Ga)As$ on the $GaAS$ substrate were obtained [16]. The two-dimensional crystals of quantum dot and antidot arrays can be also created by using the electronic lithography method.

In this report the results of calculating electron energy spectrum and wave functions are displayed for two-dimensional periodic artifitial crystals [16] placed in a strong magnetic field H. The typical value of a lattice constant has the order of 10 nm and more. It is shown that the effects of radical spectrum rebuilding defining the transport and magnetooptical phenomena must be observed in the magnetic fields equal to 1 MGs.

2. Basic equations. Calculational method

The Schrödinger equation for the electron moving in a two-dimensional square lattice placed in a perpendicular magnetic field has the form

$$\left(\hat{H}-E\right)\psi=\left\{\frac{\left(\mathbf{p}-e\mathbf{A}/c\right)^2}{2m^*}-V_0\cos^2\left(\frac{\pi x}{a}\right)\cos^2\left(\frac{\pi y}{a}\right)-E\right\}\psi=0, \qquad (7)$$

where m^* is the effective mass, $\mathbf{p}$ is a momentum. When the Landau gauge

$$\mathrm{A}=(0,Hx,0), \qquad (8)$$

is used the magnetic field H points in the z direction. The potential of the 2D-lattice in (7) (see fig.2) is described by a periodic function, therewith, the positive sign of V_0 corresponds to a quantum dot system, and the negative one to a antidot lattice. The period of such a lattice is equal to a. We suppose that the motion along the z axis is limited so that the electron is located in the lowest subband of dimensional quantization.

If p/q is a rational number the solutions of Schrödinger equation (7) must satisfy to the generalized Bloch conditions

$$\psi_{k_x,k_y}(x,y)=\psi_{k_x,k_y}(x+qa,y+a)\exp(-ik_xqa)\exp(-ik_ya)\exp(-2\pi ipy/a). \qquad (9)$$

Here the vectors of magnetic translations is chosen as follows

$$\mathbf{a}_n=n_1q\mathbf{a}_1+n_2\mathbf{a}_2, \qquad (10)$$

where n_1 and n_2 are integer numbers. Therefore, under the translation on $\mathbf{a}_n$ the wave function transforms into the function with the same values of k_x and k_y.

The solution of Eq.(7) satisfying the boundary conditions (9) may be written in the form of a series of eigenfunctions of the Hamiltonian $\hat{H}_0=\left(\mathbf{p}-e\mathbf{A}/c\right)^2/2m^*$. Such functions correspond to the spectrum

$$E_N^0=\hbar\omega_c\left(N+1/2\right), \qquad (11)$$

where N is a Landau level number. This solution of the Schrödinger equation can be written as

$$\psi_{k_x,k_y}(x,y)=\sum_{N=0}^{\infty}\sum_{n=1}^{p}C_{N,n}\sum_{l=-\infty}^{+\infty}\varphi_N\left(\frac{x-x_0-lqa-nqa/p}{l_H}\right)\exp\left(ik_x\left[lqa+\frac{nqa}{p}\right]\right)\times$$
$$\times\exp\left(2\pi iy\frac{lp+n}{a}\right)\exp(ik_yy). \qquad (12)$$

Here $x_0=c\hbar k_y/eH$, $\varphi_N(z)$ is the eigenfunction of a harmonic oscillator. The components of quasimomentum k_x and k_y are determined in the magnetic Brillouin zone.

After the substitution (12) into (7) we obtain the system of difference equations

$$\sum_{N'n'} H^{N'n'}_{Nn} C_{N'n'} = \sum_{N'n'} \left(E^0_{N'} \delta_{N'N} \delta_{n'n} + V^{N'n'}_{Nn}\left(p/q, k_x, k_y\right)\right) C_{N'n'} = EC_{Nn}, \qquad (13)$$

which defines the energy spectrum $E(k_x, k_y)$ and electronic wave functions $C_{N,n}$ .The scheme of calculation of matrix elements $V^{N'n'}_{Nn}$ is given in the Appendix. The Hamiltonian matrix $H^{N'n'}_{Nn}$ has a block structure. Each block is a three-diagonal square matrix $p \times p$. It is labeled by numbers N and N'. The number of blocks is equal to the Landau level number. The elements inside the block are marked by numbers n and n'. Therefore, the size of a full matrix is equal to $Np \times Np$. During the numerical calculations the Landau levels number N_{max} was defined experimentally so that the energy spectrum and wave functions were independent on N_{max}.

3. Results and discussion

We carried out the calculations of electron energy spectra and wave functions for a different typical parameters of two-dimensional superlattices consisting of arrays of quantum dots and antidots. The results of computations of energy spectrum for the dot lattice with a=30 nm are shown in fig.3a, 3b for different values of the magnetic field H. For the square lattice with the period a=30 nm the largest value of magnetic flux number per unit cell was $p/q = 15$. It corresponds to the magnetic field $H = 69\ T$. The depth of potential wells is equal to 300 meV and the effective mass is $m^* = 0.067\ m_e$.

Let us discuss the evolution of energy bands in the system of quantum dots and antidots in the case where the magnetic field increases. In the absence of magnetic field the levels of a single well split into the energy band and the wave functions are highly localized. Consequently, the conditions of the tight-binding approximation should be met. In a magnetic field every band splits into q subbands and the spectrum takes the form of Hofstadter's "butterfly". Such a "butterfly" produced from the lowest level of the potential well is displayed on the left side in fig.3a. The second and the third levels of the potential well are degenerated. With the increase of the magnetic field this degeneracy disappears and corresponding "butterflies" are overlapping. The system of Eqs.(13) is not periodic in p/q. Therefore, the energy band structure is also non-periodic in p/q. In the next interval $1 \le p/q \le 2$ the "butterfly" is not clearly defined.

With the increase of the magnetic field the localization of wave functions in the wells becomes stronger. Simultaneously, the transfer integrals which define a width of the energy bands in the tight-binding approximation are decreases. It leads to the narrowing of energy bands formed from the levels of a single well. We can see this in fig.3b. which prolongs fig.3a to the range of higher magnetic fields where $p/q > 2$. At the region of negative and positive energies, very narrow bands are being formed with increasing the magnetic field. These bands are clustered to the unperturbed Landau levels. Their location is marked by thick points in fig.3b.

The energy in every subband is a function of quasimomentum components k_x and k_y. In fig.4 the energy bands $E(k_y, k_x = 0)$ are shown. The component k_y is changed in the Brillouin zone (parameters of the well are the same as in fig. 3a, 3b). At the top of this figure the location of unperturbed Landau levels is displayed. At the bottom of fig.4 the parabolic dot levels in the presence of a magnetic field are plotted.

The energy spectrum of the lattice with the parameters a=10 nm, V_0=300 meV is displayed in fig.5. In this case, the following pequliarities of electron energy spectrum should be mentioned. In higher magnetic fields when $V_0/\hbar\omega_c << 1$ the nearly-free-electron approach may be used. Under these conditions the interaction between different Landau levels is not significant and the spectrum consists of subbands formed from a single Landau level. It is easy to see that in the range of magnetic fields corresponding to $p/q \ge 4$ every Landau level splits into p subbands. The energy changes in a single subband when the quasimomentum runs all values in the magnetic Brillouin zone: $-\pi/qa \le k_x \le \pi/qa$; $-\pi/a \le k_y \le \pi/a$.

In fig.6 the function $E(k_y, k_x = 0)$ is shown for different subbands formed from the Landau levels. The parameters are the same as in fig.5, but the magnetic field corresponds to $p/q = 15$. It is necessary to stress that the location of a level depends on k_y very weakly. This is as it should be since the parameter $V_0/\hbar\omega_c << 1$ and the width of the subband is exponentially small. With the increasing of Landau level's number the total width of the band decreases.

The electron energy spectrum for the antidot lattice (a=10 nm) is pictured in fig.7 with respect to magnetic field. The potential shape is the same as for the dot lattice but the amplitude has a negative sign (V_0=-300 meV). In strong magnetic fields ($p/q \geq 5$) the spectrum consists of narrow subbands which are clustered near the position of Landau levels. In the magnetic field corresponding to $p/q = 10$ the parameter $\hbar\omega_c/V_0 = 2.5$. Therefore, the structure of the energy spectrum here is the same as in the weak-binding approximation. The amount of subbands is equal to p. The location of unperturbed Landau levels is labeled by thick points.

Now let us discuss the electron eigenfunctions. The probability density corresponding to the quantum state from the lowest energy subband (see fig.4 ($p/q = 7$)) is shown in fig.8. The wave functions are localized in the quantum wells. All distributions have the lattice symmetry but at the bottom of the well the probability density has the cylindrical symmetry. The shape of this function depends weakly upon k_x and k_y. The probability density for the second energy band (see fig.4) is pictured in fig.9. We can also clearly see the lattice symmety of probability distribution but such a function has a zero point at the center of the well.

The probability distribution corresponding to the lowest energy band for a dot superlattice under $p/q = 10$ at the conditions of fig.5 is shown in fig.10. The energy of this state is positive, however, the function is mainly localized in the dot area. One can be seen the translation symmetry of the probability density. The electron density in an antidot lattice for the highest state splitted from the first Landau level is shown in fig.11. The flux quanta number here is equal to 10 and the parameters are the same as in fig.10. The structure of the wave functions pictured in fig.10 and fig.11 is similar to the one of impurity states in the field of attractive and repulsive potentials in a strong magnetic field.

4. Conclusion

The results of this paper permit to determine the range of magnetic fields and parameters of lattices in which it is possible to observe quantum effects dealing with the spectrum rebuilding of the Bloch electron in a magnetic field $H \geq 1$ MGs. In order to calculate the oscillating thermodynamical and kinetic solid state effects it is necessary to compute the density of states and the energy under the fixed concentration of carriers. It will be done in the next paper.

This research was made possible thanks to financial support from the High School Commitee of Russia (Grant 95-0-5, 5-63) and Russian Foundation for Basic Research (Grant 96-02-18067a).

Appendix

Let us discuss the scheme of calculation of the matrix elements $V^{N'n'}_{Nn}$ of the periodic potential

$$V(x,y) = -V_0\left[\cos^2\left(\frac{\pi x}{a}\right)\cos^2\left(\frac{\pi y}{a}\right)\right] \tag{A.1}$$

in the basis (12). The potential (A.1) can be written in the form

$$V(x,y) = -\frac{V_0}{4}\left[1 + \cos\left(\frac{2\pi x}{a}\right) + \cos\left(\frac{2\pi y}{a}\right) + \cos\left(\frac{2\pi x}{a}\right)\cos\left(\frac{2\pi y}{a}\right)\right]. \tag{A.2}$$

1. The calculation of matrix elements of $\cos\left(\frac{2\pi x}{a}\right)$ reduces to the definite integral

$$\int_{-\infty}^{+\infty} \cos\left[\frac{2\pi}{a}\left(l_H\xi + x_0 + \frac{nqa}{p}\right)\right] \varphi_N(\xi)\varphi_{N'}(\xi)d\xi, \tag{A.3}$$

which has been computed in [17].

2. The matrix element of $\cos\left(\frac{2\pi y}{a}\right)$ determines the transitions for k_y on $\pm\frac{2\pi}{a}$. This one is governed by the following expression

$$\frac{1}{2}\left[\delta_{n',n+1} + \delta_{n',n-1}\right] \exp\left(ik_x \frac{qa}{p}(n-n')\right) \int_{-\infty}^{+\infty} \varphi_N\left(\frac{x - x_0 - nqa/p}{l_H}\right) \varphi_{N'}\left(\frac{x - x_0 - n'qa/p}{l_H}\right) dx, \tag{A.4}$$

which is defined as the sum of two integrals

$$\int_{-\infty}^{+\infty} \varphi_N(\xi)\,\varphi_N(\xi \pm \alpha)d\xi. \tag{A.5}$$

Such definite integrals have been evaluated in [17].

3. In order to calculate the matrix elements of the product of cosines in (A.2) let us consider the auxiliary integral [1]

$$I_{N'N}(\alpha,\beta) = \int_{-\infty}^{+\infty} \varphi_N(\xi)\,\varphi_{N'}(\xi - \alpha)\exp(i\beta\xi)d\xi. \tag{A.6}$$

Differentiating the expression (A.6) with respect to α and β and using the prorerties of Hermite functions the last integral can be written as

$$I_{N'N}(\alpha,\beta) = \exp\left\{\frac{i}{2}\left[\alpha\beta + 2(N' - N)\arcsin\frac{\alpha}{\gamma}\right]\right\} \phi_{N'N}(\gamma), \tag{A.7}$$

where $\gamma = \sqrt{\alpha^2 + \beta^2}$. The integral $\phi_{N'N}(\gamma)$ depends only upon the single parameter γ and equals

$$\phi_{N'N}(\gamma) = \int_{-\infty}^{+\infty} \varphi_N(\xi)\,\varphi_{N'}(\xi)\exp(i\gamma\xi)d\xi. \tag{A.8}$$

The value of the last integral is given in [17].

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ELECTRON STATES IN PERIODIC NANOSTRUCTURES SUBJECTED TO A STRONG MAGNETIC FIELD

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Fig.1. Hofstadter's "butterfly". Electronic spectrum calculated for a square lattice with regard to magnetic flux quanta number per unit cell p/q.

Fig.2. Two-dimensional periodic potential $V(x,y) = -V_0 \cos^2(\pi x/a)\cos^2(\pi y/a)$ corresponding to a square lattice.

Fig.3a. Electron energy spectrum in a square lattice in a magnetic field. The negative range of energy is shown. The parabolic dot levels are pictured at the bottom of this figure. Such a parabolic well approximates the periodic potential $V(x,y)$ when $x \to 0, y \to 0$. The vertical variable is the number of magnetic flux quanta per unit cell (a=30 nm, V_0 =300 meV).

Fig.3b. Energy spectrum for a square lattice in a magnetic field (a=30 nm, V_0 =300 meV). The position of Landau levels in the absense of periodic potential is marked by thick points.

Fig.4. The relationship between energy E and k_y under the fixed parameter $k_x = 0$. Tne number of magnetic flux quanta passing through a unit cell (a=30 nm) $p/q = 7$.

Fig.5. Energy spectrum for a quantum dot system (a=10 nm, V_0=300 meV) in strong magnetic fields ($2 \le p/q \le 10$). The location of unperturbed Landau levels is labeled by thick points.

Fig.6. Energy band structure for a square lattice of quantum dots (a=10 nm, V_0=300 meV) in a magnetic field. $p/q = 15$, $H = 620\ T$.

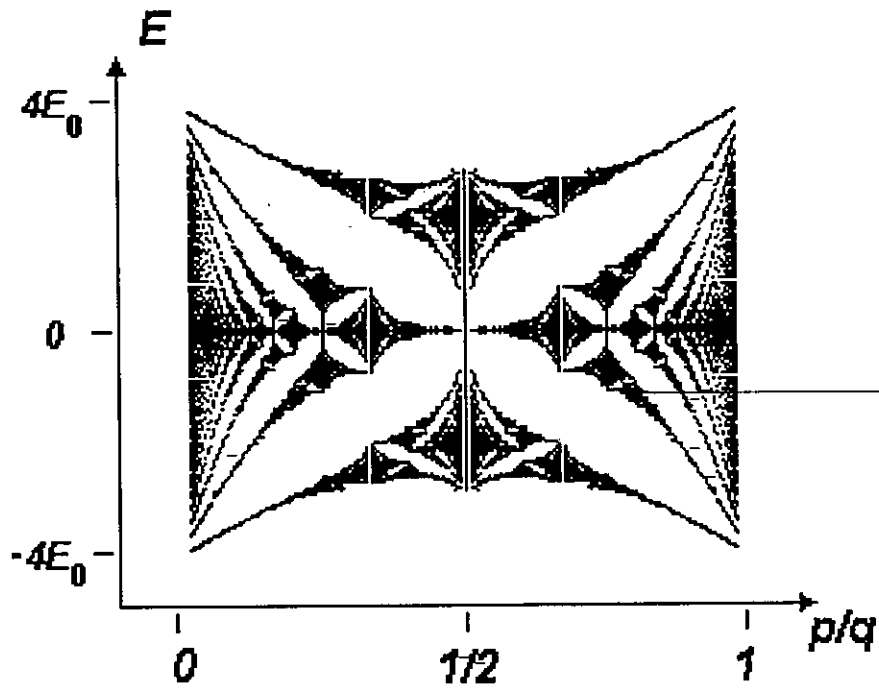
Fig.7. Electronic energy spectrum for an array of quantum antidots (a=10 nm, V_0=-300 meV).

Fig.8. The probability density in a quantum dot system corresponding to the electron state in the first (lowest) subband plotted in fig.4.

Fig.9. The probability density in a quantum dot system corresponding to the electron state in the second subband in fig.4.

Fig.10. The probability density in the quantum dot system for the electron state with the lowest energy displayed in fig.5 when $p/q = 10$.

Fig.11. The probability density in the antidot lattice for the electron state with the highest energy under the conditions of fig.7. Here $p/q = 10$.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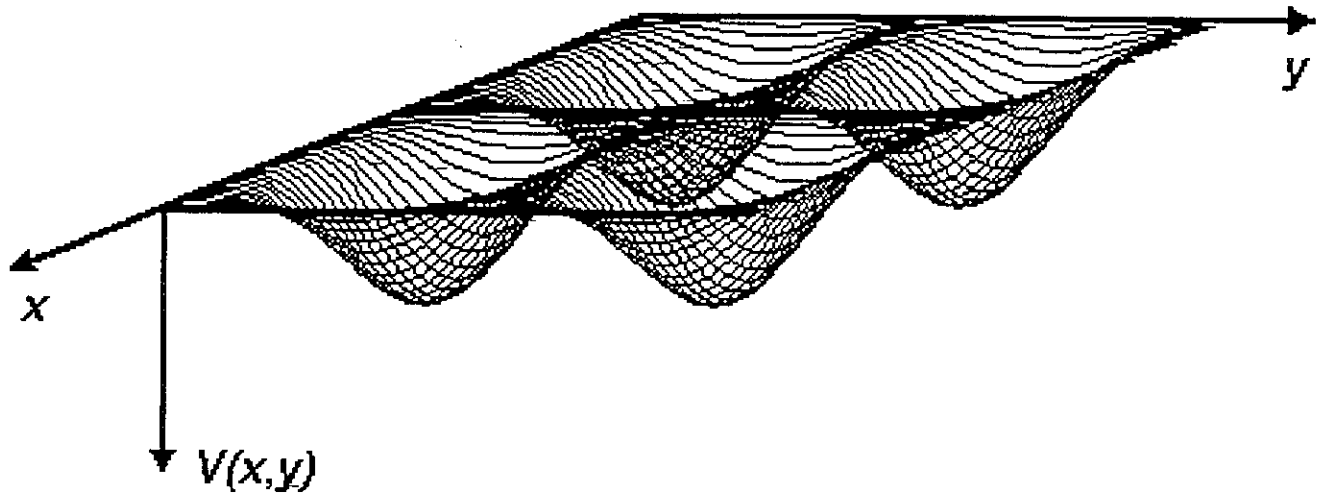
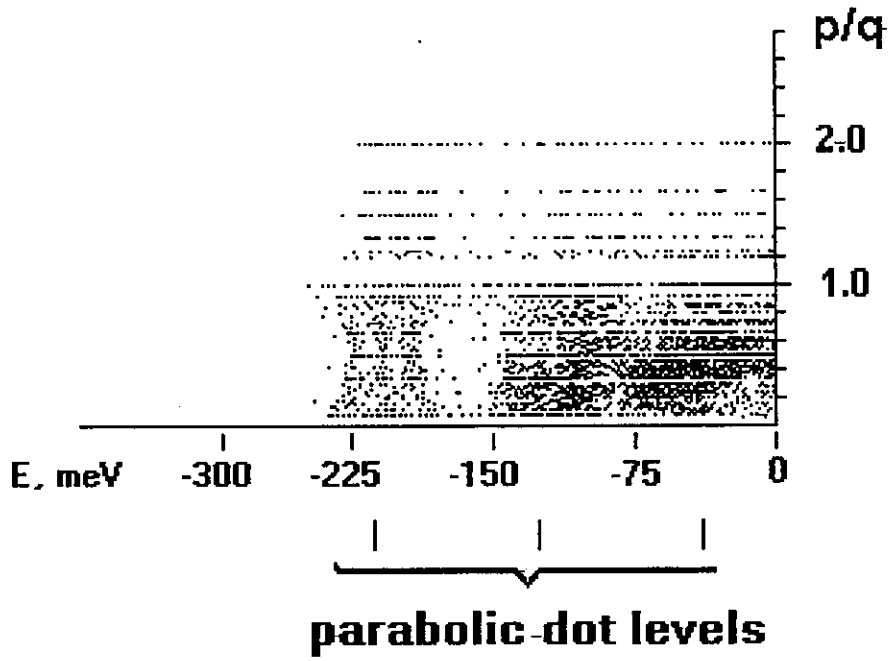
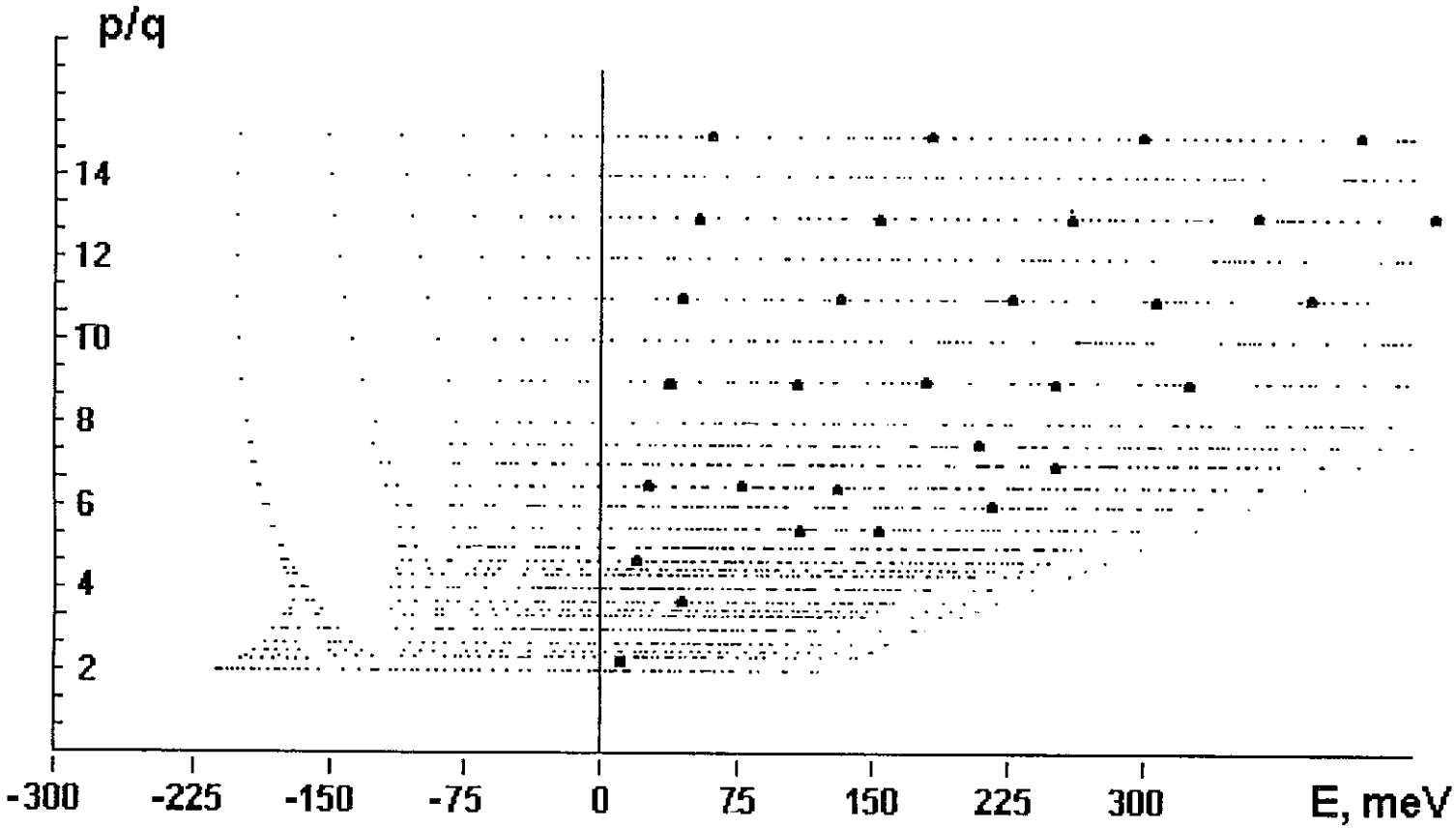
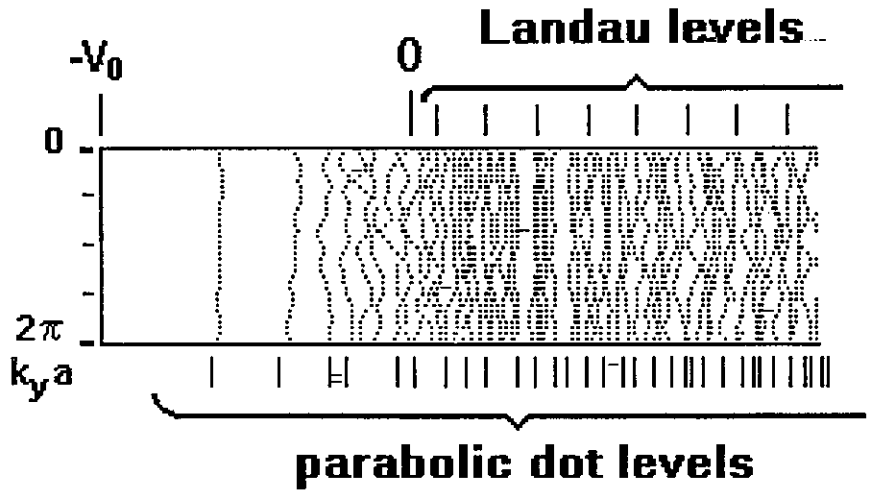
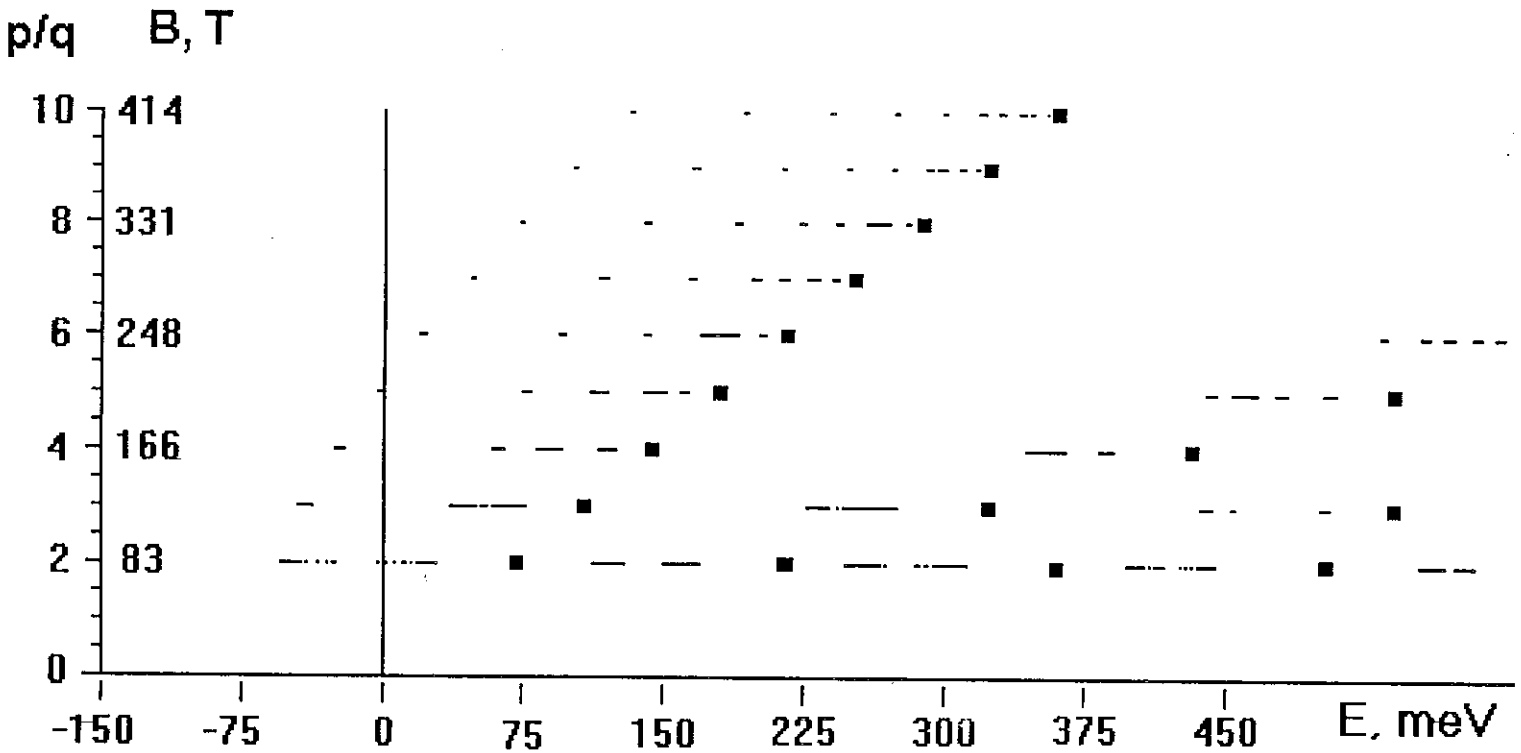
0
1/2
1
p/q


y
x
V(x,y)

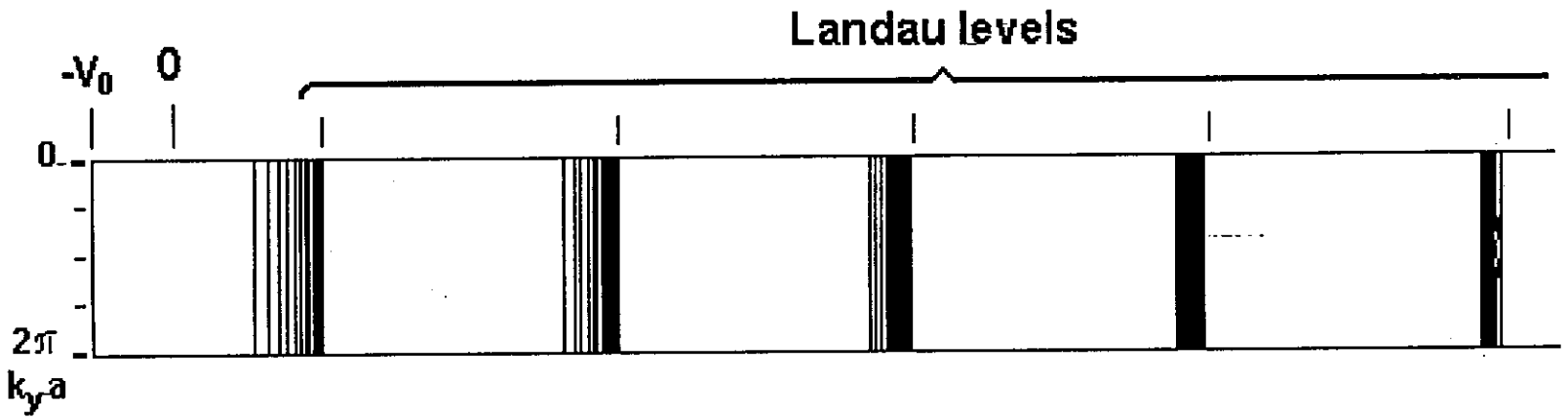

p/q
2.0
1.0
E, meV
-300
-225
-150
-75
0
parabolic-dot levels

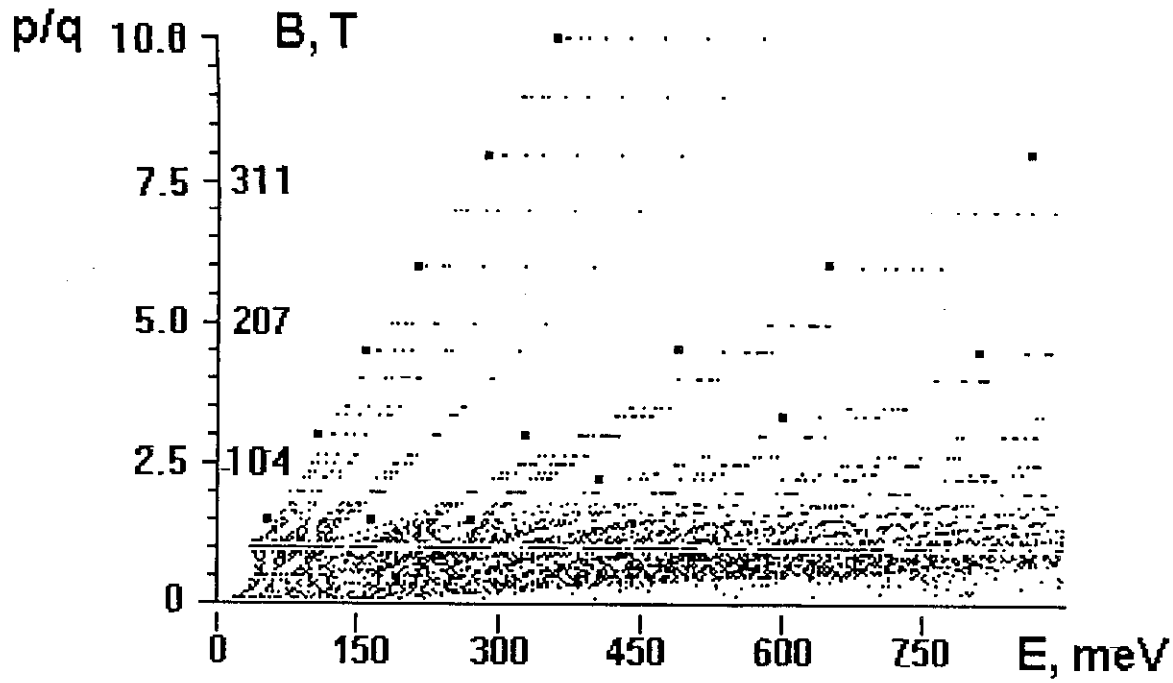

p/q
14
12
10
8
6
4
2
-300
-225
-150
-75
0
75
150
225
300
E, meV

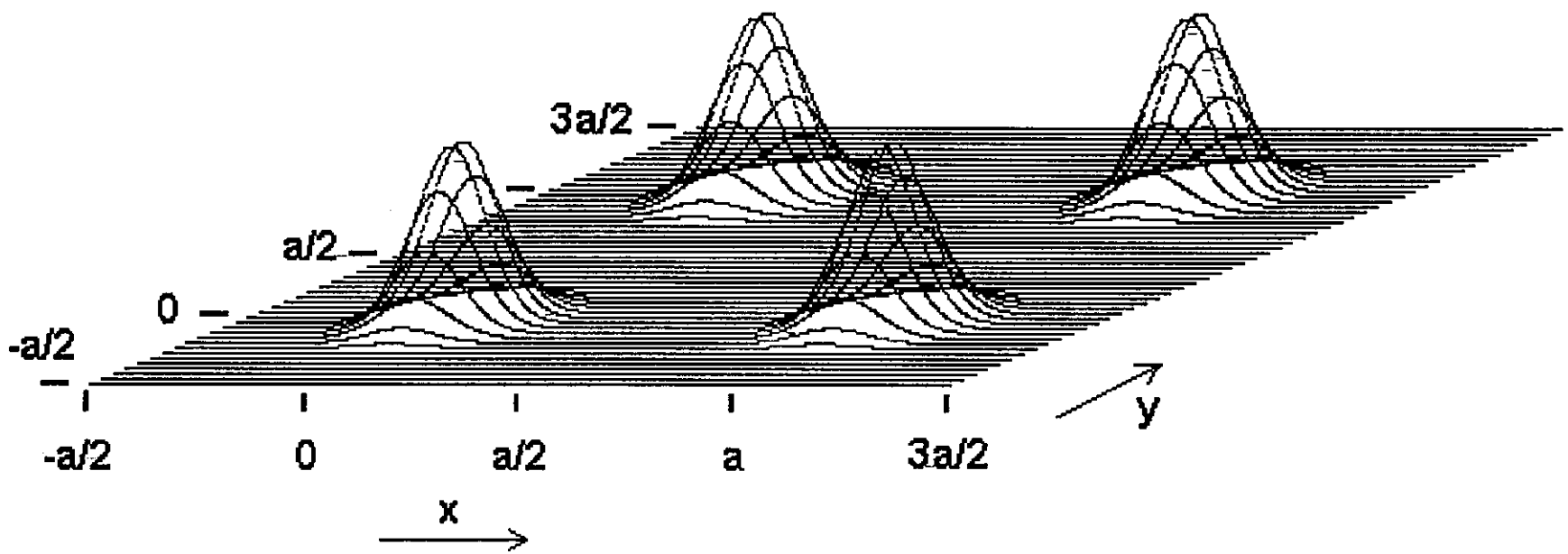

Landau levels
$-V_0$
0
0
2π
$k_y a$
parabolic dot levels

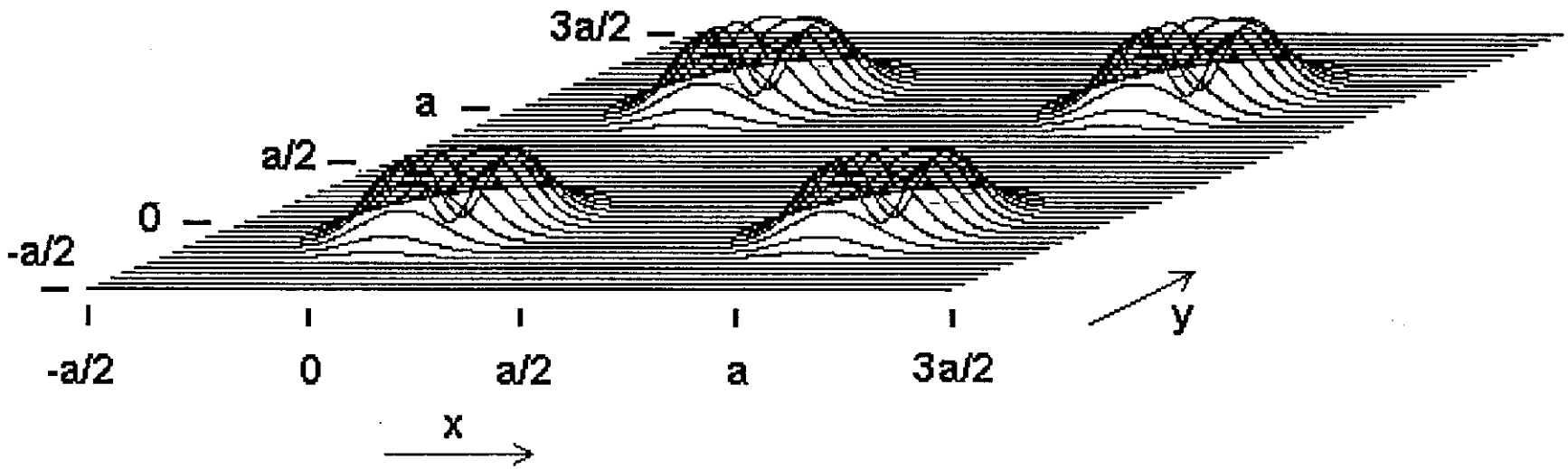


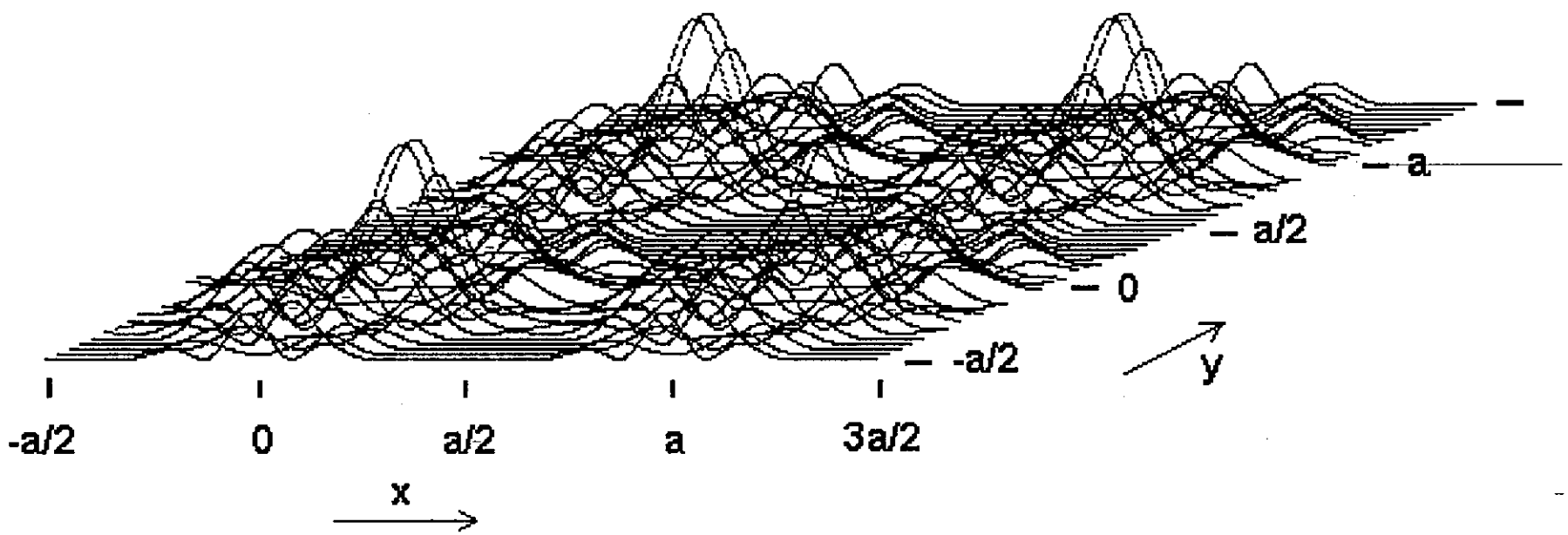
$\Delta E \sim \hbar/\tau_{rel} \sim 0.6$ meV

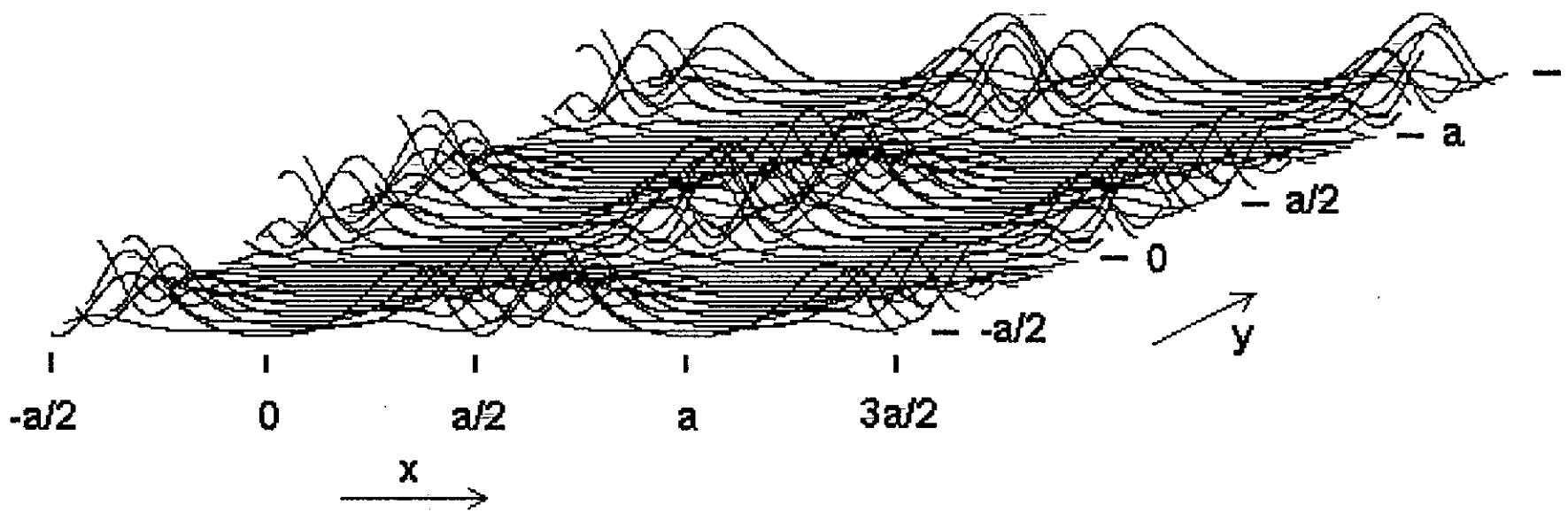

Landau levels
-V0
0
0
2π
kya


p/q
10.0
B, T
7.5
311
5.0
207
2.5
104
0
0
150
300
450
600
750
E, meV


3a/2
a/2
0
-a/2
-a/2
0
a/2
a
3a/2
x
y


3a/2
a
a/2
0
-a/2
y
-a/2
0
a/2
a
3a/2
x


-a/2
0
a/2
a
3a/2
x
-a/2
0
a/2
a
y


a
a/2
0
-a/2
y
-a/2
0
a/2
a
3a/2
x