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LETTER TO THE EDITOR

On the motion of a wave packet in a model lateral superlattice potential

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Abstract. A numerical integration of the time-dependent Schrödinger equation is used to investigate the motion of an electron wave packet under the influence of a model two-dimensional antidot array potential at zero temperature. It is shown that the motion is strongly modified by a transverse magnetic field in the regime where the magnetic length is similar to the antidot lattice constant. The intensity distribution shows that the wave function exhibits a number of complex forms. Transport in this regime is discussed in the light of the results.

Semiconductor heterojunctions in which the freedom of a two-dimensional electron gas (2DEG) is curtailed by the imposition of a periodic repulsive scattering potential have been termed lateral surface superlattices or, more simply, lateral superlattices (LSLs) [1]. Experimental measurements in this type of mesoscopic system have revealed a number of features which are not observed in the unmodulated 2DEG, namely, additional peaks in the magnetoresistance at low field [2]. These features have been explained in terms of a decrease in electron mobility associated with magnetic fields at which the classical cyclotron orbit of electrons encompasses certain integer numbers of antidots comprising the lattice [3]. If the cyclotron orbit diameter and antidot lattice constant, a, are comparable, then periodic orbits of varying form around a single antidot are possible [4]. Such models employ classical or semiclassical approximations in which a 'billiard-like' electron is scattered in some fashion by the externally imposed potential. In a transverse magnetic field the electron may be viewed as executing a skipping orbit around or between antidots [5], its trajectory perhaps becoming chaotic in some cases. In contrast to electrons in periodic orbits which are said to be 'pinned', electrons with chaotic trajectories can traverse the entire area of the antidot lattice. Pinned electrons are not able to respond to an applied electric field and make no contribution to the conductance: it is possible to estimate experimentally the fraction of carriers for which this is the case, the result being in the region of 10–20% [6].

It is the purpose of this letter to describe the results of a numerical simulation within a model which relaxes the assumption that the width of the electron wave packet is small on the scale of the antidot lattice spacing. For a typical experimental situation (where a is some hundreds of nanometres) in low or moderate magnetic fields this approximation is quite reasonable and the classical dynamics holds good. However, the approximation will fail at high fields, where quantum mechanical effects are important. An effective approach to the solution of the dynamics of an electron wave packet of finite width under

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the influence of an external potential is provided by the numerical integration of the time-dependent Schrödinger equation. It will be shown that at different applied magnetic fields the motion of the wave packet is modified in a interesting manner. The influence of the observed behaviour on the transport properties of a device in the high-field regime where the magnetic length is a significant fraction of the antidot lattice constant (where a is perhaps some tens of nanometres) is discussed. It is in this regime that Hofstadter [7] demonstrated the existence, in theory, of a self-similar energy spectrum for electrons. Whether this can be observed in a real system as one moves from the classical to the quantum mechanical regime remains something of an open question.

The Hamiltonian for the single-electron system under consideration is $\mathcal{H} = \epsilon_F = (p - eA)^2/2m^* + V_{ext}(x, y)$, where an effective-mass approach has been adopted. For the present calculation it is convenient to employ the symmetric gauge $A = (-By/2, Bx/2, 0)$ corresponding to a transverse magnetic field strength B. A square antidot lattice is considered [8], for the purposes of which a continuous model external potential of the same form as that of [3] is used, namely,

$$V_{ext}(x, y) = V_0[\cos(2\pi x/a)\cos(2\pi y/a)]^\beta. \tag{1}$$

In this model, the steepness of the potential is controlled by the parameter β, while V_0 represents the maximum value of the potential at the centre of the antidots. We also follow [3] in choosing the value of V_0 in such a way that the ratio of the antidot diameter at the Fermi energy to the superlattice spacing is one third, so as to mimic a typical experimental situation. A value of $\beta = 16$ is used throughout, giving rise to a reasonably large space between antidots in which the potential may be considered to be negligible.

In view of the fact that we wish to investigate the analogue of the classical cyclotron orbit, it is appropriate to make use of an initial wave packet of annular form. To this end, we start by considering eigenfunctions for an electron occupying the lowest Landau level in a potential-free two-dimensional system subject to transverse magnetic field B [9]. In the symmetric gauge and polar coordinates this is written as

$$\Psi_\alpha(r, \phi) = (2\pi\alpha! l_B^2)^{-1/2} e^{-i\alpha\phi} e^{-r^2/4l_B^2} (r^2/2l_B^2)^{\alpha/2} \tag{2}$$

where we have introduced the magnetic length $l_B = \sqrt{\hbar/eB}$. The width of the wave packet is of order l_B, increasing from l_B as α increases from zero. For this wave function the orbital angular momentum is quantized according to $L_z = \hbar\alpha$ where $\alpha = 0,1,2\ldots$. For the desired annular form, it is easily seen that we must have the quantum number $\alpha > 0$. Furthermore, it is readily established that the squared intensity of the initial function is a maximum at a radial distance $r_0 = \sqrt{2\alpha} l_B$ from the origin. In what follows B_0 is defined so that $r_0 = a/2$ for a given α, that is, the initial wave function has maximized intensity midway between adjacent antidots.

The time propagation scheme used is one based on an expansion of the time evolution operator $\exp[-i\mathcal{H}t/\hbar]$ as a truncated series of Chebyshev polynomials, following Tal-Ezer and Kosloff [10]. This scheme has the advantage of being able to accommodate a Hamiltonian containing magnetic field terms in an efficient manner. At time $t = 0$ the centre of the initial annular function is arranged to be coincident with the central antidot potential maximum. The parameters described above for the potential and initial wave packet ensure that there is only a small overlap between them. The system is allowed to evolve on for a time that is reasonably long on the scale of the classical cyclotron orbit period $T_c = 2\pi m^*/eB$.

Figure 1(a) shows a schematic contour plot (plan view) of the potential described by (1); it can be seen that the antidot lattice appears relatively 'open', that is, the potential is

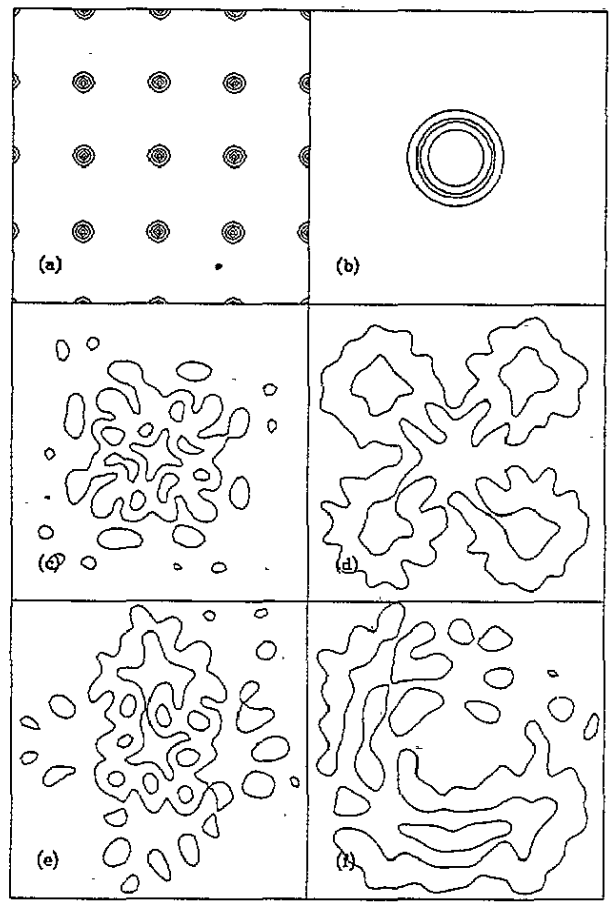

Figure 1. A contour plot of the potential described by (1) with $\beta = 16$ is shown in (a). Superimposed on this one should imagine the initial wave packet, the squared intensity of which is shown in (b). The squared intensity of the final wave function after a time $15T_c$ is plotted for various values of the parameter B/B_0: (c) 1.0, (d) 0.9, (e) 0.8, and (f) 0.7.

negligible over much of the area. Superimposed on the external potential one must imagine the initial wave packet which has an annular form, the squared intensity $|\Psi(r, \phi)|^2$ of which is shown in figure 1(b). In the examples shown the orbital angular momentum quantum number is chosen to be $\alpha = 2$, so B_0 corresponds to a magnetic length $l_B = a/4$. The remaining figures 1(c)–(f) show the propagated wave function at a time $t = 15T_c$ in an applied field of B for differing values of B/B_0.

Figure 1(c) depicts the situation for $B/B_0 = 1$. Here, we can see that the initial wave function has been scattered to some extent by the antidot lattice but retains much the same form (compared with $t = 0$) in that the majority of the intensity remains in the region around the central antidot. (It should be noted that the integrated norm over the whole area of the wave function remains constant in time, as expected.) The central minimum of the final wave packet is still present, but small, while there is some evidence of a build-up of intensity in the potential free region diagonally between antidots. If the value of l_B (and consequently r_0) is increased then, as one would expect, the initial wave function is scattered to a greater extent [11]. It is necessarily the case that the rotational symmetry

of the initial situation should be preserved, as both wave function and potential share this symmetry around the central antidot. That some small asymmetry appears in the result after $15T_c$ is due to a residual asymmetry introduced by the discretization of the problem on a finite grid and is ignored as we are interested in the more general, large-scale, features. However, the growth of such asymmetry could be taken as an indication of the stability of the solution.

The value of B/B_0 is now reduced so that, in the classical picture, an electron tends to take up a cyclotron orbit of greater diameter than that for $B/B_0 = 1$. The result is shown is figures 1(d) and 1(e) where B/B_0 is equal to 0.9 and 0.8 respectively. The final wave function in both these cases shows a markedly different form to that seen in figure 1(c) for $B/B_0 = 1$. In 1(d) it can be seen that areas of high intensity form a striking geometric pattern around the scattering centres in positions diagonally opposite the central antidot, while in 1(e) the final wave function is more concentrated about the four nearest-neighbour antidots. If B/B_0 is reduced further to 0.7 as in figure 1(f) the final wave function shows no definite pattern. More intensity moves towards the sides of the grid box which suggests that the wave function is not constrained to move about the central antidot as in (d) and (e); a larger grid is required to see if any larger-scale pattern evolved as it is possible that propagation becomes unphysical in this calculation as significant intensity reaches the edge of the grid.

The pinning orbits envisaged in the classical models where the cyclotron orbits encircle integer numbers of antidots are all essentially circular in character. The present results show that such a picture is clearly inadequate when l_B becomes a significant fraction of a. Considerably more complex orbits may be imagined in this case, enclosing a larger number of antidots over a wider area. It is possible that electrons in these more complex orbits will remain pinned when an electric field is applied, as suggested by the forms seen in (d) and (e). A large number of different patterns of this type are conceivable if the number of antidots is increased giving rise to more possibilities for pinning. In this way one would see the suppression of the classically chaotic motions exhibited by the billiard model, which is characteristic of a quantum mechanical system. This would clearly be reflected in the fine structure of the observed magnetoresistance via the removal of mobile electrons following chaotic trajectories.

There are a number of factors which are not included in the calculation at this time, where we have considered a single-electron wave packet moving in a square lattice. Different lattice geometry or disordered lattices [12] could easily be studied within the present approach but, owing to the nature of the propagation scheme, the modelling of the Coulomb repulsion in a many-electron system would be more problematic. However, it has been shown [13] that the time-dependent approach is efficacious in the calculation of properties more directly related to experiment in two dimensions, namely the conductance. It is clear that the finite width of the electron wave packet is important and should be addressed when devices become small enough that $l_B \sim a$ at moderate magnetic fields.

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