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QUANTUM OPTICS IN SEMICONDUCTOR HETEROSTRUCTURES[1]

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In this paper we show examples where dynamical processes in semiconductor heterostructures are integrated. Systems and devices are chosen where two degrees of freedom are involved.

1. Introduction

The operation of many recent semiconductor devices is derived from the technical ability to design space structures of desired form [1]. Such mesoscopic heterostructures provide simple realizations of many model systems treated in quantum mechanics textbooks. Thus they also offer researchers the opportunity to investigate fundamental processes displayed by the charge carriers in the material. These can be manipulated by doping, thermal excitation or external carrier injection. The present situation thus offers a wide range of phenomena which are of interest from a fundamental point of view but which are also relevant for the technical development of the field.

The technical devices operate over ever shorter time scales and smaller space distances. They are thus genuinely time dependent and steady state properties do not provide all the information needed to understand the phenomena involved. The passage of electronic wave packets through the structures gives an excellent opportunity to determine the space and time scales characteristic of the various stages of a complicated time evolution. Experimentally it is still not possible to launch and follow single electron wave packets coherently, but the theoretical calculations allow this. They have thus turned out to provide a transparent tool for the research into dynamic phenomena in semiconductor heterostructures [2].

The numerical integration of the time dependent Schrödinger equation is, however, far from trivial even with modern computers. In particular, the numerical effort grows rapidly with the number of degrees of freedom; thus one can reasonably easily carry our

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calculations in one dimension, but the addition of further degrees of freedom rapidly exhausts the computer resources. This we first encountered in adding spontaneous decay to the molecular wave packet dynamics [3]. In this paper we give an overview over some simple semiconductor situations where the investigations have required the integration of two-dimensional time evolution.

In Sec.2 we review the physics of single electron quantum dynamics in a semiconductor. In spite of the simplicity of the formulation, the full complexity of a solid structure lies below. Thus the wave functions that obey a Schrödinger-like wave equation are envelope approximations based on the fundamental Bloch states of the structures. Thus it is only a crude first approximation, but we cannot here go into the considerations required to justify it.

In Sec.3 we present the theory of a simple two-electron device where the motion of one charge is gated by the arrival of the other one. In Sec.4, a one-dimensional electron is emitting light when passing through a suitably designed barrier structure. This provides the basis for a coherent micro-cavity laser, and the single lasing mode gives the second degree of freedom. Finally in Sec.5 we integrate the motion of a single electron through a genuinely two-dimensional structure. In this situation we can imitate the diffraction processes encountered in ordinary optics; hence we call this conduction electron optics. The examples presented are only offered as illustrations; for the details of the systems and the numerics, the readers are referred to the original publications.

Finally the results are summarized and some omissions and simplifications are presented in Sec.6. In this paper we cannot, however, go into any details concerning the possible extensions of the discussion.

2. Time dependent envelope approach

In bulk solids, a single electron basis is given by the Bloch states

$$b_{s,\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}\, u_{s,\mathbf{k}}(\mathbf{r}), \tag{1}$$

where s denotes the band index, $\mathbf{k}$ is the lattice momentum, and $u_{s,\mathbf{k}}(\mathbf{r})$ has the symmetry of the lattice. The energy in the band s is given by a function $\varepsilon_s(\mathbf{k})$. In a pure semiconductor crystal, the bands are either filled (valence bands) or empty (conduction bands) at zero temperature. At finite temperatures, the size of the band gap determines the amount of thermally excited conduction electrons, which leave behind them holes carrying positive charges.

In a semiconductor heterostructure, layers of different materials are sandwiched in consecutive layers, so that large sheets of pure material are separated by parallel interfaces. This creates a structure which is homogeneous in two directions (x and y say) but changes abruptly from one material to another in the third (z) direction. The material parameters change over a few atomic layers only. A simple example is shown in Fig.1, where a material II is sandwiched between bulk samples of another material I. The lower part of the figure shows how the conduction and valence bands acquire spatial variation in their energy.

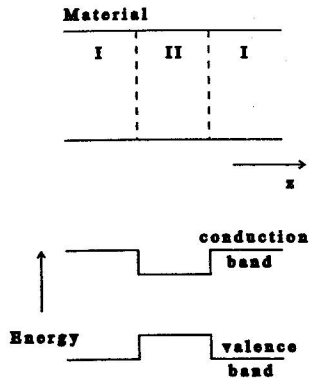

Fig. 1. The semiconductor heterostructures consist of layered materials (I and II) with different band gaps.

In a structure of the type discussed above, the electrons see bulk properties in the transverse (x and y) directions and hence the states can be taken to be of the form (1). In the z–direction, the state takes a different shape. In the time dependent case, we assume that we can separate the dynamics in the z–direction from the transverse degrees of freedom. Thus we write

$$\Psi(\mathbf{r},t) = \sum_s \varphi_s(z,t)\, \exp\left[i(k_x x + k_y y)\right]\, u_{s,\mathbf{k}}(\mathbf{r}). \tag{2}$$

The function $\varphi_s(z,t)$ is the envelope wave function. Its time evolution is taken to derive from the bulk energy $\varepsilon_s(\mathbf{k})$, when the k_z–dependence is expressed in the position representation. In the bulk case (1), the relation between $\mathbf{x}$ and $\mathbf{k}$ is like a Fourier transform, and hence we can approximately replace k_z by $-i\frac{\partial}{\partial z}$ as in ordinary Quantum Theory. This function is, however, different in each band and each material [4]. Using the properties of the Bloch states, we obtain the approximate time evolution equation for the envelope function

$$\begin{aligned} i\hbar\tfrac{\partial}{\partial t}\varphi_s(z,t) &= \varepsilon_s^y(-i\tfrac{\partial}{\partial z})\varphi_s(z,t) \\ &= \left[\varepsilon_s^y(0) - \tfrac{\hbar^2}{2m_s^y}\tfrac{\partial^2}{\partial z^2} + \ldots\right]\varphi_s(z,t). \end{aligned} \tag{3}$$

The index y signifies the material ($y = I$ or II). The latter form introduces the band effective mass m_s^y which makes the equation look like a Schrödinger equation. The potential function $\varepsilon_s^y(0)$ gives a constant value for each material indicated by y. In this way, we obtain a quantum problem in a layered structure. We are going to discuss the dynamics of semiconductor electrons in this approximation; the theory for holes is exactly similar. The various electron bands indicated by the index s are assumed to be coupled by external optical field exactly as in the bulk situation.

The theory suggested by the argument above is a first approximation only. Its validity should be estimated and the corrections should be evaluated. In this paper we do, however, not address these difficult questions. We are satisfied to accept (3) as our starting point and evaluate its consequences.

3. A two-electron device

Real electrons are affected by many interaction processes in a semiconductor. A central feature is their mutual Coulomb repulsion. The quantum nature of the particles also manifests itself in the symmetry or antisymmetry of the wave function. The simplest system where we can investigate such phenomena consists of two electrons. We choose to carry out such an investigation on a device where the motion of the one electron is gated by the presence of the other one [5]. Their interaction takes place in a heterostructure shown in Fig.2, where the barrier height is taken to be $V_0 = 0.115\,eV$. The sequence of potential barriers is chosen such that near the energy $E = 0.754\,V_0$ the particles are transmitted and near $E = 1.20\,V_0$ they are reflected; this is shown in the lower part of Fig.2.

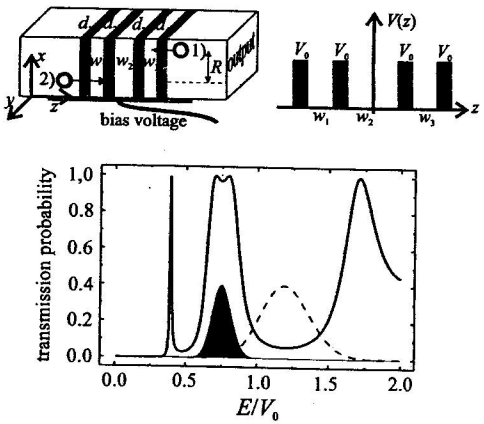

Fig. 2. The upper part of the figure (left) shows a schematic picture of the structure used for the two-electron gate. The right side gives the potential barriers: they have $d = 33$ Å and the wells are $w_1 = w_3 = 33$ Å and $w_2 = 55$ Å. This leads to the transmission profile in the lower part. The shaded and the dashed profiles are the energy ranges of the incoming wave packets.

The device is operated in such a manner that electron 1 is launched from the right with its energy in the pass region (shaded energy distribution in Fig.2) and electron 2 is launched from the left with energy in the reflection region (dashed energy distribution in Fig.2). If the electrons were independent particles, they would both emerge to the left. However, when electron 2 enters the barrier region, it will occupy the potential wells for a while, and the electron 1 will be reflected by the repulsive interaction. In the ideal case it will emerge out in the right direction. The current emerging to the right is thus gated by the arrival time of electron 2. In the quantum case it makes no

sense to state which electron goes which way; in fact we can even get out more than one electron to the right.

Electrons are Fermions, but we can also use our model system to investigate the influence of quantum statistics. The two-electron system time evolution occurs in the one dimension (z) which is transverse to the barriers. We can satisfy the antisymmetry of the electron states by the function along the barriers. This emerges if we write the three-dimensional state in the form

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, t) = \Phi(z_1, z_2, t)\,\eta(y_1, y_2, x_1, x_2). \tag{4}$$

All time dependence is ascribed to the motion in the $z-$direction. This ansatz is inserted in the two-electron Schrödinger equation for the envelope function, and we integrate over the $x-$ and $y-$coordinates. Thus we end up with the effective equation

$$i\hbar\frac{\partial}{\partial t}\Phi(z_1, z_2, t) = \sum_{i=1}^{2}\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z_i^2} + V_B(z_i)\right)\Phi(z_1, z_2, t) + \overline{V(|\,z_1 - z_2\,|)}\,\Phi(z_1, z_2, t), \tag{5}$$

where $\overline{V(|\,z_1 - z_2\,|)}$ is the Coulomb interaction averaged over the function $\eta(y_1, y_2, x_1, x_2)$. By choosing this to be symmetric or antisymmetric in the two electrons, we can use an antisymmetric or symmetric initial state for the function $\Phi(z_1, z_2, t)$; we refer to these as the Fermion or Boson case respectively.

When the particles are considered classical, the operation of the gate can be described as in Fig.3, upper part. In the $z_1 - z_2$ plane the barrier structure is situated at $z_1 = z_2 = 0$ and the particle interaction is at $z_1 = z_2$. The electrons are launched from $\{z_1, z_2\} = \{+\infty, -\infty\}$. In the case labelled (+), the electron 2 reaches the barriers first, it is reflected and the electron 1 passes the barrier without being affected; both electrons emerge in the direction $\{-\infty, -\infty\}$. Likewise in the case labelled (-), when the electrons meet to the left of the barriers. In the case (0), however, the two electrons occupy the barrier structure simultaneously and their repulsion deflects the electrons in the direction $\{+\infty, -\infty\}$. Thus the arrival time of the electron 2 gates the fate of the electron 1.

The lower part of Fig.3 shows the result of wave packet integrations of Eq.(5). Here we have not yet introduced the symmetry of the wave packet; this corresponds to classical electron statistics. As can be seen, the centres of gravity of the electronic wave packets behave very much like the ideal trajectories drawn in the upper part of the figure. Thus the gate is expected to operate as designed. This is verified in the part (a) of Fig.4. When the two wave packets are launched so that they reach the barrier structure simultaneously, nearly one electron is reflected to the right. If they are launched so that they are separated by about twice their width (=400 Å) the amount scattered falls to about 0.2 electrons. This is the gating operation we are looking for. In Part (a) we have chosen the relative dielectric constant ε of the medium equal to unity. Then the Coulomb interaction is strong, and dominates the behaviour; no effect of the statistics can be seen. We can soften the electron-electron interaction by introducing a larger dielectric constant. Part (b) increases this to $\varepsilon = 2.2$, which is enough to bring out the effect of the symmetry. The gating action is less for the Fermions, because they

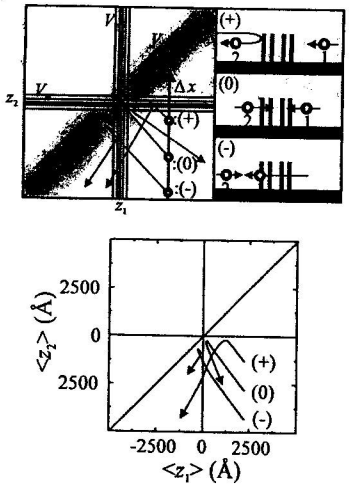

Fig. 3. The upper part shows how the gate operates with classical particles. In the cases (+) and (-) both electrons are found to emerge to the left. In the case (0) one electron is scattered back to the right. The lower part shows the centre of mass motion of a wave packet where the particles have kept their identities (classical case).

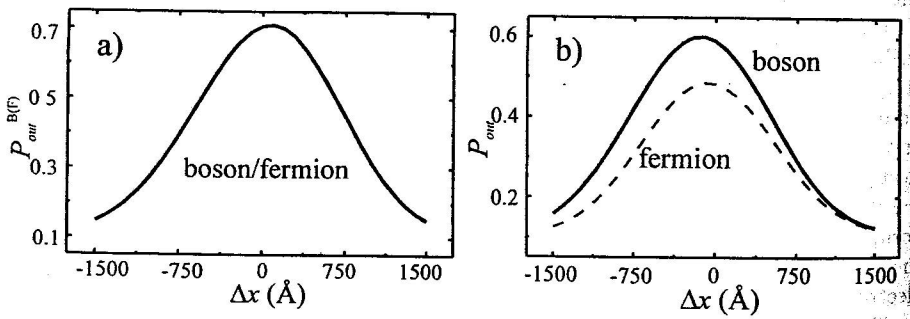

Fig. 4. The backscattering probability as a function of delay between the wave packets. In part (a), $\epsilon = 1$ and the symmetry does not affect the result. In (b) the interaction is made weaker by setting $\epsilon = 2.2$ and the statistics can be discerned.

tend to avoid coming close, and thus the Coulomb repulsion is less efficient in turning around the one electron.

We have seen that the two-electron gate works as we designed it. The Coulomb interaction can be used to steer the course of the electrons when the resonant structure of the barriers is utilized. The symmetry of the wave function can also be seen as it affects the gating action. For more details about the choice of model and its parameters the reader is directed to the original publication [5].

4. Micro model of a cascade laser

The semiconductor electron laser designed by Capasso [6] still operates in a regime where many electrons contribute incoherently to the amplification of the laser light. In this Section we report on a micro-laser version of the quantum cascade laser. Following the micro-maser and micro-laser work, we look at a structure where the gain is contributed by a coherent interaction between a single electron and a single micro cavity mode [7]. By letting the electron tunnel through a heterostructure, we can utilize photon assisted tunnelling processes to transfer electronic band energy into photons. Because the electron propagates coherently, we can utilize the resonances inside the structure to tune the emission, and the whole process can be made fast. It is found to occur over time scales of the order of less than $1\,ps$. Because the electronic relaxation processes have been found to take about $4\,ps$, the emission process can be considered as the traversal of a wave packet through the structure.

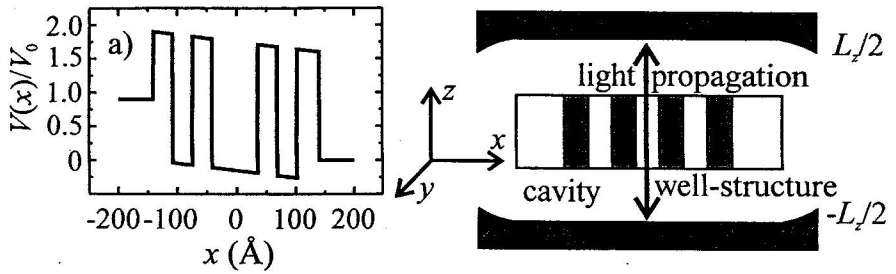

Fig. 5. In part (a) the potential structure used in the cascade laser; on the right is shown how it is situated in a laser cavity.

The heterostructure chosen is shown in Fig.5. The doping of the material is combined with a suitable bias to achieve the barrier structure shown to the left. To the right is shown a schematic picture of the semiconductor material inside an optical cavity. We assume that this can be operated in a single optical mode. The whole volume of the cavity is about $0.5\,\mu m^3$, which implies a micro cavity.

The system is described by the following Hamiltonians: The electrons propagate in the x–direction through the layered barrier structure according to the Hamiltonian

$$H_{el} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x), \tag{6}$$

and the field mode is described by

$$H_{field} = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right) = -\frac{\hbar^2}{2M_f}\frac{\partial^2}{\partial Q^2} + \frac{1}{2}M_f\omega^2 Q^2, \tag{7}$$

where we have used the field coordinate Q as defined via the use of a fictitious field mass M_f according to

$$Q = \sqrt{\frac{\hbar}{2M_f\omega}}\left(a + a^\dagger\right). \tag{8}$$

Using the second form of (7), we integrate the mode degrees of freedom as if they were mechanical variables. This gives directly the wave function of the photon state in the cavity.

The interaction between the electron and the cavity mode is taken in the minimum coupling formulation to be

$$V_{int} = -\frac{e}{m}\mathbf{A}\cdot\mathbf{p} + \frac{e^2}{2m}\mathbf{A}^2 = -i\hbar\Lambda Q\frac{\partial}{\partial x} + \frac{1}{2}m\Lambda^2 Q^2, \tag{9}$$

where the coupling constant is given by

$$\Lambda^2 = \frac{M_f}{m}\left(\frac{e^2}{m\varepsilon_0 V}\right) \tag{10}$$

as follows from the standard expansion of the vector potential $\mathbf{A}$ in terms of the field coordinate Q. The coupled equations (6)-(9) define a standard Schrödinger problem with two degrees of freedom. Assuming an electron wave packet entering the structure from the left and a suitable initial state for the cavity mode, we can integrate out the subsequent time evolution and look at the exchange of energy between the electron and the cavity mode.

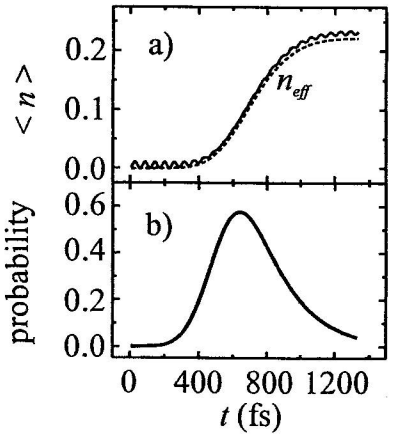

Fig. 6. Part (a) shows how the photon number is increased from vacuum during a single electron event. The wiggles are free-electron oscillations in the field. Part (b) shows the occupation probability of the heterostructure. We can see that the tail decays approximately exponentially.

In Fig.6 (a) we start with the cavity in the vacuum state. The electron enters the barrier structure, with some probability it tunnels and emits a photon. In the case shown, this happens with probability 0.23; thus each electron leaves behind 0.23 photons. This is the single process gain of the device. In part (b) of the figure, we show the probability for the electron to be found inside the barrier structure. It penetrates, and it subsequently leaks out in a nearly exponential manner as suggested by [8]. The

whole process is, however, over after 1000 fs as was stated earlier. The state of the cavity mode is written in the form

$$|\,field\rangle = C_0\,|\,0\rangle + C_1\,|\,1\rangle. \tag{11}$$

The vacuum and single photon probabilities $|\,C_0\,|^2$ and $|\,C_1\,|^2$ are shown as functions of time in Fig.7.

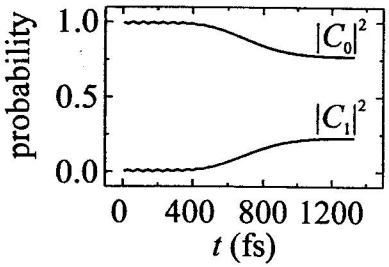

Fig. 7. The behaviour of the vacuum amplitude C_0 and the one photon amplitude C_1 during the single interaction event. As we can see, the process is completed in 1 ps.

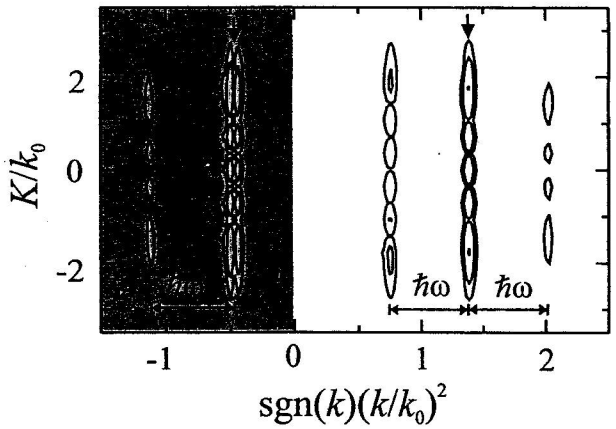

Fig. 8. The wave function of the combined single electron and the cavity mode. Both are given as functions of their energies expressed in terms of the wave vectors. The electron energy is plotted separately for transmitted components (positive energy) and reflected components (negative energy). The electron wave components are separated by the photon energies $\hbar\omega$.

We can also look at the gain in the laser cavity when it is initially not empty. We choose to display the two-dimensional electron-photon wave packet in the momentum representation; K for the photon and k^2 for the electron. In this manner the scales give also the energy of the particles. For the electron we, however, multiply the k^2 by the sign of k to separate the transmitted wave from the reflected one. For the photon states the probability $|\,\langle K\,|\,n\rangle\,|^2$ has got $n+1$ maxima for the state $|\,n\rangle$.

In Fig.8 we show the final state starting from $n = 4$; this is seen both in the transmitted and the reflected waves. In the transmitted one, there is a certain probability that the field ends up in $n = 5$ (6 maxima) but then the electron energy has been decreased by the amount $(\hbar\omega)$. We also see a loss process, where the electron is accelerated but the field goes to $n = 3$ (4 maxima). The gain process is seen only after the barrier structure, the loss can occur also in reflection.

We have thus shown that the single electron can be used to feed photons into the cavity. This is micro-laser operation. If the cavity could be made to have low enough losses, the device could be operated in steady state. This is a considerable technical difficulty for a realistic material, but the basic principle has been established by these calculations. For the detailed discussion of the operation and the choice of parameters we refer to the original publication [7].

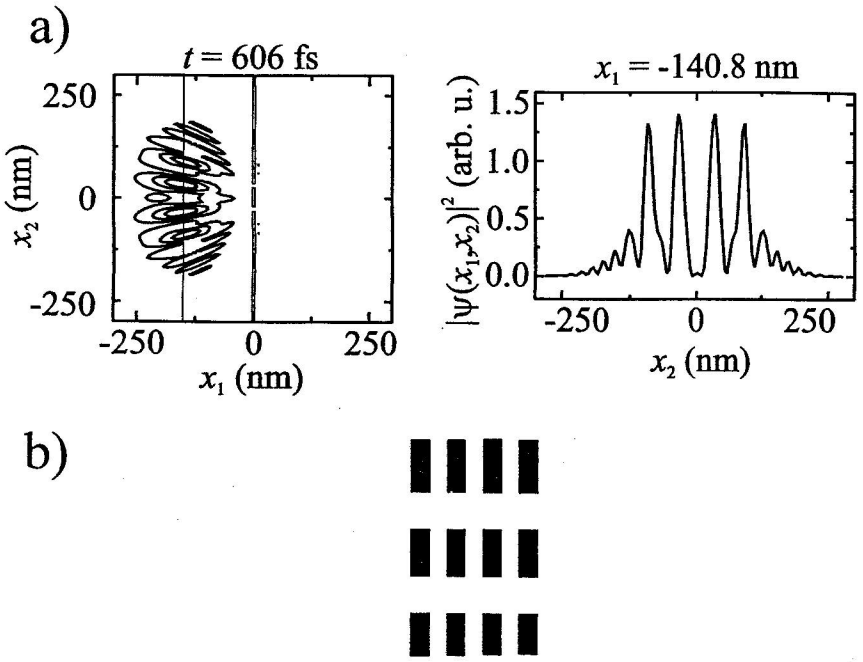

Fig. 9. A two-dimensional electron optics configuration displaying the characteristic two-slit pattern. The barrier in part (b) is the same sequence as in Fig.2, but with two penetrating holes. After the wave packet passed the barrier (at $t = 606\,fs$) the position at the dotted line shows the interference pattern shown to the right in part (a).

5. Conduction electron optics

The technology to design potential structures of arbitrary shape allows one to make beam shaping devices for conduction electrons. It is hence possible to imitate all the components of conventional optics for electronic wave functions. To illustrate the use of such artifacts, we choose the sequence of barriers given in Fig.9 (b). By selecting the electron energy in the transmission or reflection region, we can at will choose a situation where the electrons do not see the barriers or one where the structure is opaque. This corresponds to having a material with variable optical properties. Various applications are presented in our work [9]

In Fig.9 we present a single example where the structure is shaped into an electron version of the celebrated two-slit experiment; see the structure in the lower part of the figure. This configuration has played a central role in the discussion of quantum theory [10] and it has been experimentally realized by optical waves (Young's experiment), free electrons and most recently with atoms [11]. Figure 9 (a) shows that the same effect can, in principle, be achieved with the charge carriers in a semiconductor structure. The wave function is the envelope of the electronic state, but the physics remains the same. The distribution of probability in the wave packet after the slits is given by the picture to the right; it represents a cut along the dotted line in the picture to the left. In spite of the imperfections deriving from the use of a barrier structure and a finite wave packet, the familiar diffraction pattern is seen.

We have thus suggested [9] that the technology to manufacture suitably designed heterostructures gives the possibility to make integrated structures for electron optics in semiconductors. If relaxation processes can be avoided, this would provide the possibility to copy the device structures of integrated optics for the conduction electrons.

6. Conclusions

In these investigations we have found that many features of electron dynamics in heterostructures can be illuminated by the use of propagating wave packets. The computational resources available only allow two degrees of freedom to be treated, but this offers a multitude of interesting situations. Fundamental physical processes as well as idealized simple devices can be discussed.

The single electron picture used here must, however, be corrected in many ways. The Coulumb interaction leads to a genuine many-body problem, and the appearance of excitons and possibly collective oscillations complicate the picture. These effects are well understood, but this does not mean that they are easy to treat numerically. It will be a challenging task for both theoreticians and experimentalists to find out which phenomena survive in models more realistic than the ones presented here.

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