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Simulating and Visualizing the Dynamics of Coherent Quantum Transport in Strong Magnetic Fields

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Electron propagation under the influence of magnetic fields is one of the most fundamental problems in physics and engineering. Coherent electron propagation manifests itself in several quite distinct contexts ranging from electron holography and transmission electron microscopy, to 'mesoscopic' devices. Recent analysis[1, 2] of coherent electron transport in 'mesoscopic' devices has to a large extent used classical billiard ball models or semiclassical models, or solutions of the static Schrödinger equation.

As the size of research devices becomes smaller and smaller, devices using coherent electron propagation become increasingly under investigation. Examples are quantum cascade lasers, Bloch oscillators, quantum interference devices and others. Recently, great breakthroughs have also been achieved in the field of quantum computation, where quantum mechanics is used directly for computation. Thus it becomes increasingly important to be able to simulate and to visualize the dynamics of coherent electron propagation in device structures in order to develop the intuitive understanding necessary for device design.

In the present work, I present the development of a new very efficient method to simulate and visualize the dynamics of quantum transport, including strong magnetic fields. The method solves the time-dependent Schrödinger equation, including strong magnetic fields. The dynamics of electron propagation through arbitrary potentials, strong magnetic and electric fields can be simulated and visualized. I have also incorporated selfconsistency in the programs. (Preliminary results have been presented in Ref. [3], graphical results of simulations results in zero magnetic field have been awarded the 2nd Prize in the Japanese Computer Visualization Contest 1995[4])

The propagation of electron wave packets is calculated by solving the time-dependent Schrödinger equation. The wave function $\Psi(x, y, t+\delta)$ is calculated from $\Psi(x, y, t)$ at the previous time step by applying the time evolution operator U. Typically, I use grids of 1 Million pixels or more and time-steps of 1 fs.

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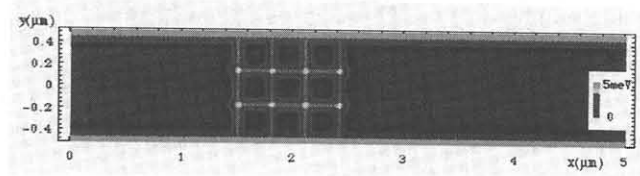

Figure 1: *Potential of the sample of Ref. [6]. Simulation results of electron propagation in this sample are visualized in Fig. 2.*

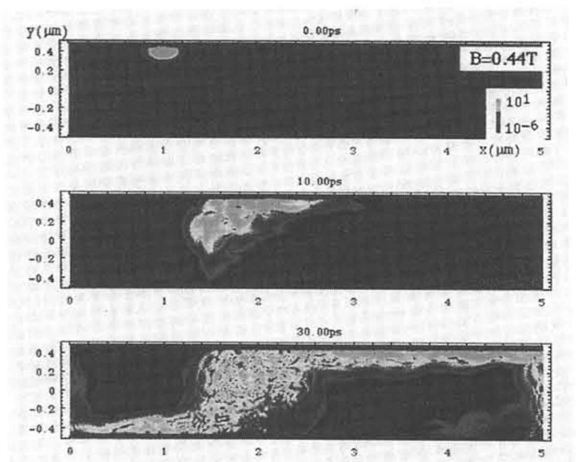

Figure 2: *Simulation of Quantum Transport through the 'mesoscopic' grid structure device of Fig. 1. Subfigures show the absolute value of the wave function at 0, 10, and 30 picoseconds after start of simulation (B=0.44 Tesla)*

Transport in 'anti-dot lattices' and other potential grids have recently been studied intensively. Practically all studies of transport in anti-dot lattices have been performed in the *classical regime*[5]. Only very recently Lenssen et al.[6] explored an anti-dot lattice in the *quantum transport regime*. Fig. 1 shows a model for the potential of the sample of Ref. [6] and Fig. 2 visualizes the flow of the electron wave function through this sample.

Figure 3 compares the measured conductance to the calculated transmission. Clearly, the major features are in very excellent agreement, however the oscillation period in the calculation differs from the measured one. Further work shows, that the remaining discrepancies in the

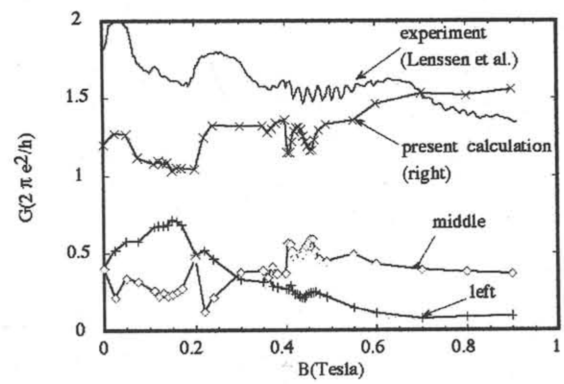

Figure 3: *Comparison of the calculated transmission with the experimental result of Ref. [6]. The integral over the absolute square of the wave function in the area to the right of the grid is related to the transmission probability. Landauer's formula shows that the conductance is related to the quantum mechanical transmission probability. The figure also shows the integrated values of the absolute square of the wave function in the area of the grid and to it's left.*

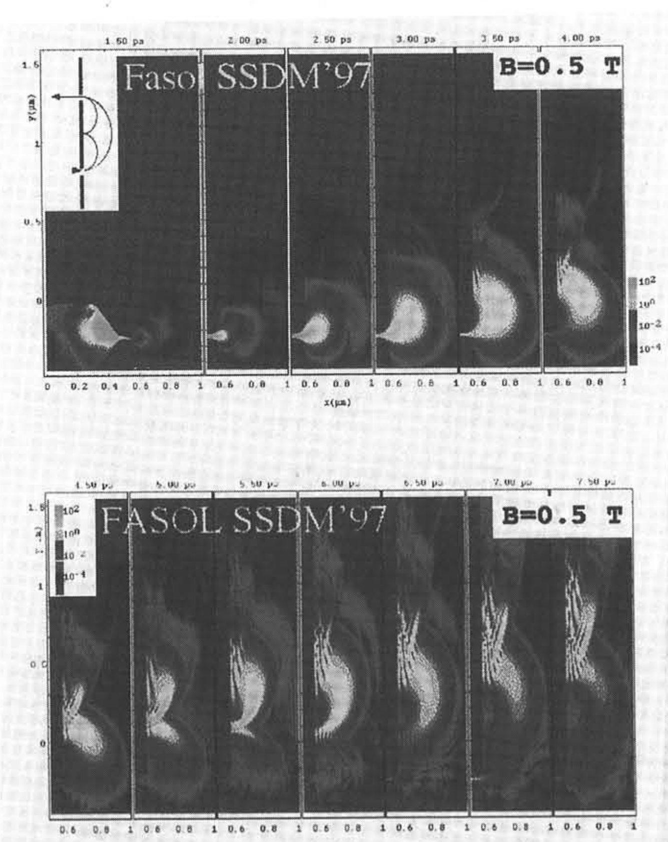

Figure 4: *Propagation of an electron wave packet through an electron focussing structure (B=0.5 Tesla).*

oscillation period can be reduced by including the self-consistent potential.

Coherent electron focusing due to magnetic fields is one of the key experiments in 'mesoscopic' transport. It was investigated by van Houten et al. and many others[2, 7] and has become a much used technique, culminating in it's recent use for the detection of composite Fermions[8]. In a classical approximation, focusing peaks are expected in the transmission probability from a first to a second point contact, at magnetic fields such that the separation between point contacts is an integer multiple of the cyclotron diameter. Note however, that previous analysis employed semiclassical methods, which are known to have severe difficulties when caustics are present.

Figure 4 shows the results of calculating the propagation of an electron wave packet through an electron focusing experiment. The simulation shows, that the character of the electron wave packet propagation crosses over from 'semi-classical' to 'quantum mechanical edge state' character with increasing time and increasing magnetic field.

In conclusion, I have introduced a method to solve the time-dependent Schrödinger equation in order to simulate and visualize the dynamics of the flow of electron wave packets through quantum devices. Such advanced simulations and visualization techniques are essential for the design of quantum devices.

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