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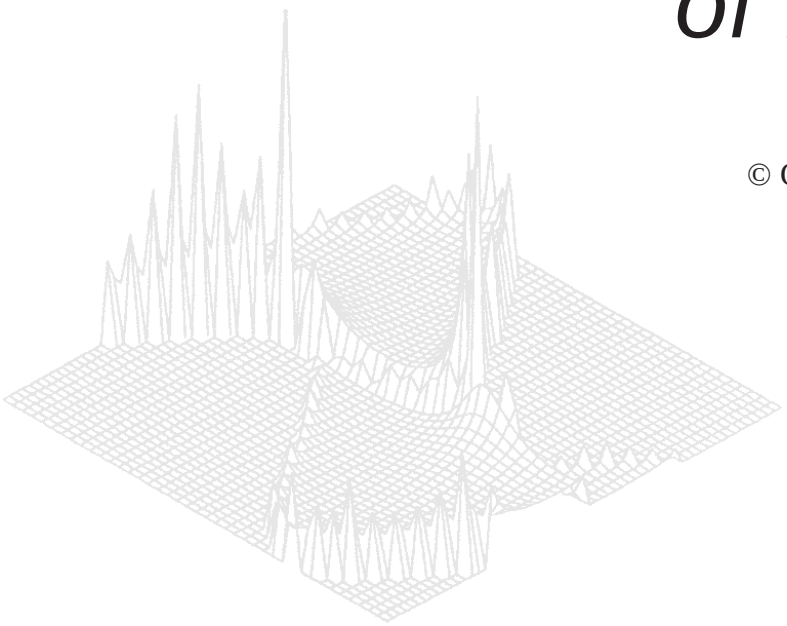

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Time-dependent Quantum Waveguide Theory: A Study of Nano Ring Structures*

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Abstract

As electronic circuits get progressingly smaller to the nanometre scale, the quantum wave nature of the electrons starts to play a dominant role. It is thus possible for the devices to operate by controlling the phase of the quantum electron waves rather than the electron density as in present-day devices. This paper presents a highly accurate numerical method to treat quantum waveguides with arbitrarily complex geometry. Based on this model, a variety of quantum effects can be studied and quantified.

1. Introduction

It is known that as electronic circuits get smaller and smaller to the nanometre scale, device analysis based on semiclassical transport theories, such as using the Boltzmann rate equation, will eventually fail. This is because the characteristic dimensions of nanometre structures are comparable to the wavelength of an electron with energy from meV to a few eV, and thus the quantum wave nature of the electrons starts to play a dominant role. For instance, the wavelength of an electron with energy 1 meV is about 40 nm. For an electron with energy of 1 eV, its wavelength is about 1·2 nm. Very recent advances in semiconductor fabrication technology have already allowed construction of mesoscopic structures from 100 nm to 1 nm in size and confined in two, one and zero dimensions [for an overview see Sohn (1998), for quantum dots see Kouwenhoven (1998), for carbon nanotubes see Tans *et al.* (1998) and for single-atom-chain nanowires see Yanson *et al.* (1998)]. These nanostructures are expected to become the building blocks of the next-generation electronics.

A pressing challenge to theory is to provide an accurate prediction of quantum transport and interference in these nanostructures, such as nonlocal effects, resonant tunnelling, Coulomb blockade, low dimensionality effects, Aharanov–Bohm interference, electron–electron correlation, and spin exchange coupling. In fact, the size of electronic components cannot be scaled down much further without properly dealing with the quantum effects that emerge on the nanometre scale. The next-generation ultra-fast computers with lower consumption and more compact circuits will need to take advantage of quantum mechanical phenomena.

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One of the possibilities is for the devices to operate by controlling the phase of a few electrons rather than the electron density as in present-day devices. In this way, less energy is required and fast switching times can be achieved. Another possibility is to establish communications between quantum wires and quantum dot cells through the nonlocality nature of the electron waves without the need of traditional wires to propagate information.

By pushing devices to such an extreme, a classical '*billiard-ball*' description of electron motion is no longer valid, and neither is a semiclassical description of electron densities via Boltzmann-type rate equations. Theoretical calculations of these device properties require a full quantum mechanical treatment. This paper aims to establish a highly accurate and effective theoretical model of nanometre scale quantum waveguides by directly solving the time-dependent Schrödinger equation

$$i\frac{\partial\psi(\mathbf{r},t)}{\partial t} = \mathcal{H}\psi(\mathbf{r},t)\,. \tag{1}$$

2. Theory

As a prototype case, we examined a nanometre-scale ring structure shown schematically in Fig. 1*a*. Such a device can be made by electron-beam lithography as described by Kane *et al.* (1998). The middle metal gate (i.e. the light grey area) is biased positively to induce conduction electrons in the semiconductor layer. The side and central gates (i.e. the dark grey area) are biased negatively to confine the conduction electrons in a narrow tunnel. The confinement potential is depicted in Fig. 1*b*. Electron transport between the source and the drain is dependent on quantum waves propagating around the ring and undergoing interference with reflections from the potential barriers. These barriers can be raised or lowered by changing the negative voltage applied to the metal gates.

The quantum-wire fabrication technique developed by Kane *et al.* (1998) eliminates the need for a dopant layer in the heterostructures adjacent to the 2D electrons. Consequently, the quantum cavity is free of impurity that may be introduced by modulation doping and thus has essentially perfect crystalline structure. Both the electron mean free path and the phase coherence length are greater than the sample dimension, and there are no holes. The conduction electron density in the nanowire can be controlled by adjusting the middle gate voltage and is typically around 10^{10} cm^{-2}, equivalent to one electron in an area of 100 nm $\times$100 nm (Kane *et al.* 1998; O'Brien 1999).

Of course there are many other electrons in the semiconductor, but the rest of them are tightly bound to the nuclei in the solid. Such nanostructures are frequently referred to as single-electron tunnelling devices, since their central channels often hold but a single conduction electron. In this case, the electron–electron correlation effect on electron transport properties is small. This independent electron approximation of mesoscopic structures is supported by many experiments (Webb 1998). Also, at low temperatures of several Kelvin, the energy of phonons is too low to interact with the electrons and often neglected (Jacak *et al.* 1998). If, in addition, the few conduction electrons in the semiconductor stay near the bottom of the conduction band during the tunnelling process and the external potential is not strong enough to induce interband transitions, the standard single-electron effective-mass approximation is then valid.

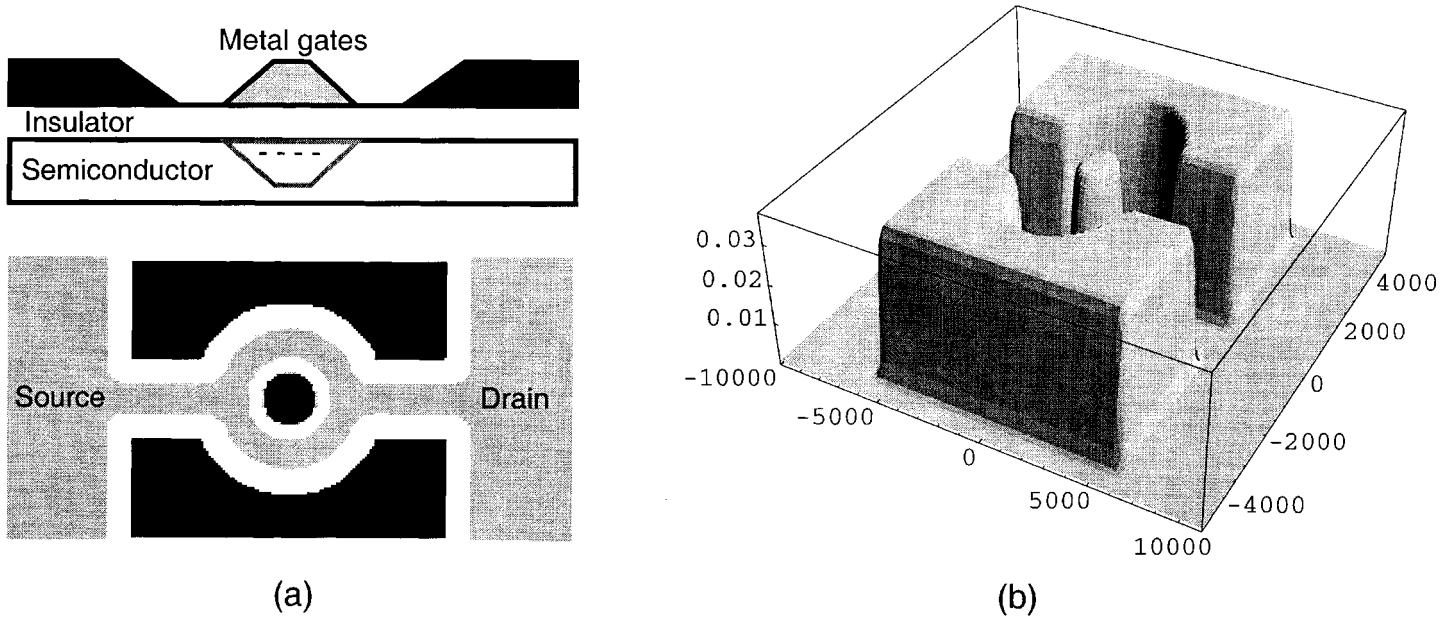

Fig. 1. (*a*) The side and top view of the device. The dark grey regions are negatively charged metal gates and the light grey area is positively charged. (*b*) The confinement potential.

Because of the interaction with the crystal lattice in the quantum wires, the conduction electrons appear to have a different mass from m_e (Tanner 1995). In this case, the time-dependent Schrödinger equation for describing a two-dimensional electron motion in the potential of the lattice plus the potential of an applied external potential $V(x, y)$ is given as

$$i\frac{\partial\psi(\mathbf{r},t)}{\partial t} = -\frac{\hbar^2}{2m^*}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)\psi(x,y,t) + V(x,y)\psi(x,y,t)\,, \tag{2}$$

where m^* is the effective mass of the semiconductor material. For GaAs, the effective mass m^* is $0{\cdot}066$ a.u.

Current theoretical work on quantum waveguides is predominantly based on the separability of time and spatial variables, which leads to the time-independent Schrödinger equation

$$\mathcal{H}\psi(\mathbf{r},t) = E\psi(\mathbf{r},t)$$

(Jin *et al.* 1999; Varshini 1998; Nikolic and Sodan 1998; Gu *et al.* 1998; Carini *et al.* 1997; Clark and Bracken 1996; Tachibana and Totsuji 1996; Popov and Popova 1996). What distinguishes nanostructure analysis from most previous applications of quantum mechanics is that boundaries often play a central role in controlling the magnitude, phase and direction of electron transport. This poses a serious challenge to conventional time-independent methods and often defies an adequate solution. In some cases, a special transformation is required to obtain simpler boundaries in the new coordinate system, but this normally gives rise to more complicated differential equations (Clark and Bracken 1996). For this reason, generally structures with very simple geometry have been studied.

The time-dependent approach aims to obtain a full solution of the time-dependent Schrödinger equation directly. The formal solution has been known for a long time as (Goldberger and Watson 1964; Taylor 1972)

$$\psi(x,y,t+\Delta t) = \exp(-\imath\mathcal{H}\Delta t)\psi(x,y,t)\,,$$

but computational techniques for treating the exponential time propagator $\exp(-\imath\mathcal{H}\Delta t)$ have been slow to develop and practical calculations have had to await the arrival of powerful computers. Different approximations to the exponential time propagator $\exp(-\imath\mathcal{H}\Delta t)$, along with the technique used to evaluate the action of the Laplacian ∇^2 on the wave function, lead to different time evolution schemes.

In an earlier publication (Wang and Scholz 1998), we discussed several time-dependent approaches including the Euler expansion, the first and second order difference schemes, the Taylor expansions, the split operator method, and the Chebyshev scheme. We applied the Chebyshev scheme to 1D potential scattering and our results were in excellent agreement with exact solutions. A comprehensive discussion on the time-dependent quantum mechanical approaches especially related to reactive scattering can be found in the review article written by Balakrishnan *et al.* (1997). We also studied 2D electron propagation through a double barrier using the Chebyshev scheme (Wang and Midgley 1999). This

paper extends our previous work to investigate electron wave propagation in a nanometre-scale ring structure.

Briefly, the Chebyshev scheme approximates the exponential time propagator by a Chebyshev polynomial expansion:

$$\psi(x,y,t) = \exp[-\imath(E_{\max}+E_{\min})t/2]\sum_{n=0}^{N} a_n(\alpha)\phi_n(-\imath\tilde{\mathcal{H}})\psi(x,y,t=0)\,, \qquad (3)$$

where $E_{\max}$ and $E_{\min}$ are the upper and lower bounds on the energies sampled by the wave function, $\alpha = (E_{\max}-E_{\min})t/2$, $a_n(\alpha) = 2J_n(\alpha)$ except for $a_0(\alpha) = J_0(\alpha)$, $J_n(\alpha)$ are the Bessel functions of the first kind, ϕ_n are the Chebyshev polynomials, and the normalised Hamiltonian is defined as

$$\tilde{\mathcal{H}} = \frac{1}{E_{\max}-E_{\min}}[2\mathcal{H} - (E_{\max}+E_{\min})]\,. \qquad (4)$$

The above normalisation ensures that the expansion of Chebyshev polynomials is convergent. Since the Bessel function falls to zero exponentially as n increases beyond α, it follows that terminating the expansion at $N > \alpha$ would yield accurate results. Note that α is proportional to the time step t and so is the number of terms required in the expansion. Since the time step t can be arbitrarily large, this scheme is often used as a one-step propagator to cover the complete interaction.

3. Results and Discussion

A major concern with such a time-dependent propagation approach is its accuracy in obtaining the final system wave function, because errors accumulated over many time steps may cause severe distortion of the wave functions. Even for one-step time propagators, such as the Chebyshev scheme used in this work, errors may accumulate when using the recursion relation to calculate the higher order terms in the expansion. The typical number of iterations range from a few hundred to several thousand. Therefore, before the Chebyshev scheme can be used to model various systems, the scheme needs to be checked against a set of criteria.

First of all, the norm of the wave function must be conserved throughout the time-evolution since there is no loss of flux anywhere. This test is very effective in verifying the model because the Chebyshev scheme is not unitary by definition. Consequently, if the norm is preserved it is a good indication that the expansion is accurate. Secondly, since we are dealing with closed systems, the energy should also remain constant. This is a basic requirement of quantum mechanics. Thirdly, consistency under time reversal is another requirement of quantum mechanics. If the wave function is propagated for some time and then propagated backward in time to its original position, any significant numerical error will cause the final wave function to be different from the initial one. Consistency under time reversal is extremely sensitive to numerical errors.

The potential chosen to demonstrate compliance with the above tests is shown in Fig. 1*b* The height of the potential walls is $3\cdot 676\times 10^{-2}$ a.u., while the space spanned by the potential is 20000×10000 a.u. The incoming electron has a

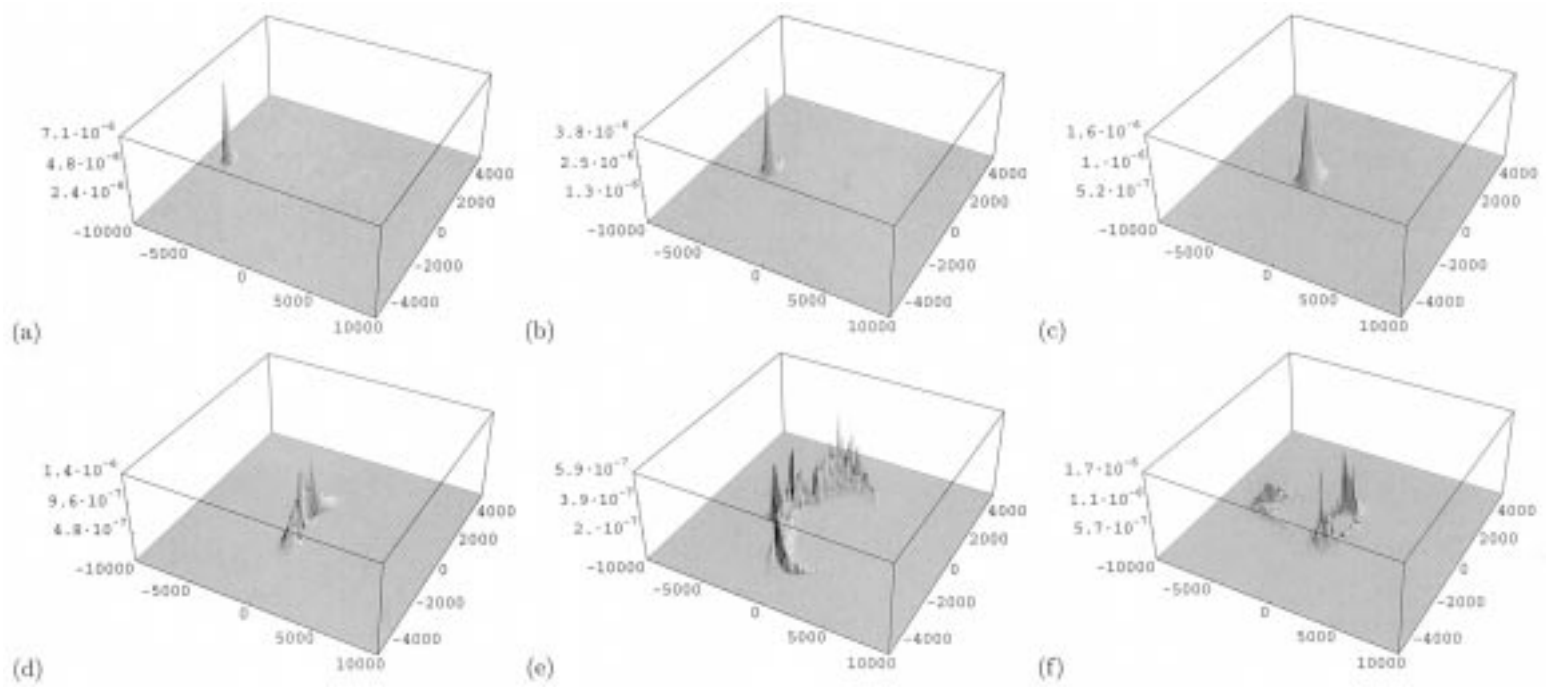

Fig. 2. Propagation of the wave function through the potential: (*a*) the initial wave function and (*b*)–(*f*) the wave function at the end of each time step.

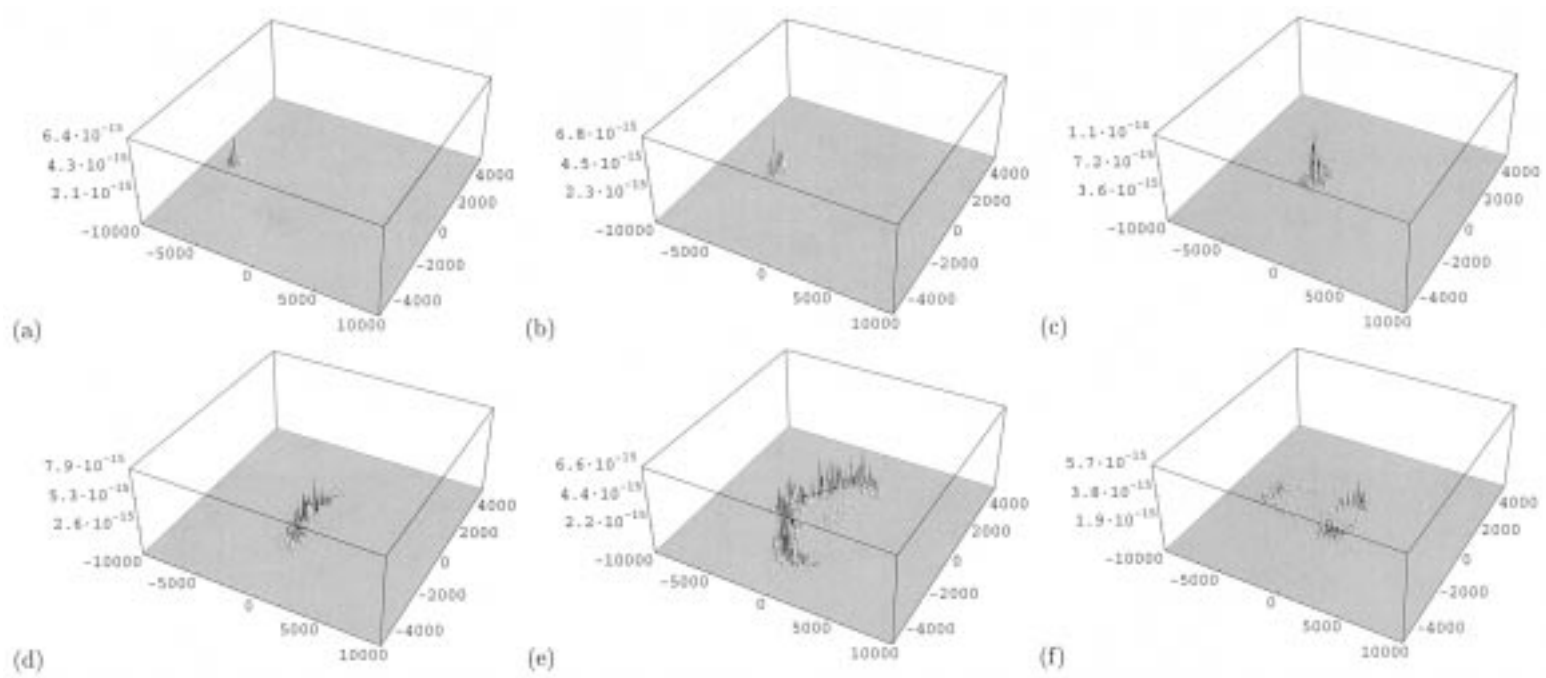

Fig. 3. Error between forward and reversed propagation: (*a*) the error between the initial and the final time-reversed wave function and (*b*)–(*f*) the error between the wave function at the end of each time step and the wave function propagated backwards to the same time.

dominant energy of $3{\cdot}0 \times 10^{-2}$ a.u. with a spread in momentum of $7{\cdot}5\%$. The width of the propagation channel is 2000 a.u. and the radius of the ring is also 2000 a.u. The total time of propagation is $0{\cdot}1687 \times 10^5$ a.u., which was split up into six equally spaced time steps of $0{\cdot}2812 \times 10^4$ a.u.

The propagation of the wave function is shown in Fig. 2. Part (a) is the initial wave function with (b)–(f) showing the wave function at the end of each time step. As shown, the wave function travels along, hits the middle pole of the ring, and part of the wave function reflects from the pole with the rest propagating around it.

Fig. 3 shows the error between the wave function propagated forward in time and the wave function propagated backward in time to the same position. This error is the difference between the two wave functions divided by the maximum value of the forward propagated wave function. Part (a) is the error between the initial wave function and the returned wave function. Parts (b)–(f) show the error between the forward wave function and the wave function propagated back to the same position. As can be seen the error is about 10^{14} times smaller than the amplitude of the corresponding wave function, indicating that the propagation scheme is extremely accurate and self-consistent.

Throughout the propagation, the relative change in the norm of the wave function and the relative change in energy of the system were both of the order of 10^{-14}. The comparison with the known solution of free space propagation is also extremely good and the error is approximately 10^{-16}, which is of the order of the machine accuracy (double precision). The addition of a non-zero potential introduces negligible error, but the computational time and working arrays increase due to the requirement of a finer grid.

The amount of memory required to perform the above calculations was 87 MB and the grid size was 1176×420 (which corresponds to 493,920 double precision complex numbers or $7{\cdot}5$ MB of memory for each array). The total time for the calculations was approximately $1\frac{1}{2}$ hours on a 500 MHz Digital Personal Workstation (Alpha processor) with 256 MB of memory. The derivatives required for the Hamiltonian were computed using the Fourier transform method (Wang and Scholz 1998) using the FFTW package.*

Since the wave function contains complete quantum mechanical information about the system under study, we can derive from it all possible observables such as the reflection and transmission coefficients, the lifetime of trapped states, resonance, interference, and phase shifts. The energy spectrum (or the density of states) can also be obtained from the time propagation of system wave functions by using the time–energy Fourier transform. In this way, one can filter out intensity weighted spectra from the correlation function defined as the overlap integral of the wave function at time t with the initial wave function (Feagin 1994; Tomsovic and Heller 1993).

4. Conclusion

The Chebyshev scheme provides a very powerful tool to model the propagation of electrons through arbitrarily shaped quantum waveguides. This scheme can be readily applied to examine many different types of systems. Of interest are

* The FFTW package was developed at MIT by Matteo Frigo and Steven G. Johnson, see http://www.fftw.org.

conductance fluctuation in nano wires, trapped states in bent nano wires, resonant tunnelling through barriers, and many more. The introduction of electric and magnetic fields is also straightforward. This model can be further extended to include deformation of confinement potentials due to the transport of electrons, which is a real effect in experimental work.

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