Parallel algorithms for the simulation and visualisation of interacting few-electron quantum transport in laterally patterned low-dimensional semiconductors

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Abstract

A parallelised Chebyschev accelerated over-relaxation algorithm is developed for simulating the few electron problem inhigh magnetic fields. A novel form of resonant tunnelling is proposed to occur through a single potential barrier due to the confining potential provided to one electron by a following electron in quasi-one dimensional current flow.

I. Introduction

Arrays of coupled ultra-small capacitor structures exhibit significant charging effects due to the large charging energies deriving from the small values of the components of the capacitance matrix. In particular, the occurrence of single-electronic effects such as the Coulomb blockade, correlated single-electron tunnelling, and the demonstration of switchable single flows, has raised hopes of a future single-electronics technology. The "orthodox model"[1] of correlated single-electron tunnelling has been highly successful for the relatively large metal-insulator systems; it assumes continuous energy distributions, large numbers of states in the 'metallic' electrodes and simplified pictures of tunnelling and electron correlation. However, many tenets of the orthodox theory are lost in the 2DEG semiconductor systems and in the recently proposed coupled Schottky dot structures[2]. Rather than a single electron picture we must deal with a *few-body problem* in which only distant dense 'electrodes' might be treated by self-consistent mean field approaches.

Previously[3,4,5] we have developed a vectorised algorithm for the numerical modelling of 2D quantum transport through quantum point contact structures, quantum waveguides and Aharonov Bohm ring devices using the ADI algorthm on the discretised 2D Schrödinger equation. This method fails for high magnetic fields due to errors arising from non-commutativity of the split kinetic energy operators. It is also unacceptable in accuracy for the few body problem and regions of complex quantum chaos.

II. Algorithms

This work is part of a much more general problem which concerns the modelling of the transport of *n-interacting electrons* within an arbitrary shaped quantum waveguide (hence discrete energy states) including *charging effects*. Our algorithm has been structured such that the interacting 2 electron problem can be studied for a 1D spatial model. The 2 electron problem in configuration space is isomorphic to the problem of 1 electron in 2D space in the presence of an effective 2D potential given by the sum of the confinement potentials for each electron plus the Coulomb potential. Consider first the 1 electron 2D time-dependent Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\psi(x,y,t) = H\psi(x,y,t) \qquad (1)$$

which has solutions of the form

$$\psi(x,y,t) = \psi(x,y,0)\exp\left\{-\frac{iHt}{\hbar}\right\} \tag{2}$$

or

$$\psi(x,y,t+\Delta t) = \psi(x,y,t)\exp\left\{-\frac{iH\Delta t}{\hbar}\right\} \tag{3}$$

Using the Cayley Expansion for the exponential and defining $\tau = \frac{i\Delta t}{2\hbar}$

$$\psi(x,y)^{t+1} = \psi(x,y)^{t}\frac{1-H\tau}{1+H\tau} \tag{4}$$

Where the t indices refer to discrete time.

Now for a single electron two-dimensional system with time-independent potential profile the time-independent Schrödinger Equation is given by

$$H\psi(x,y) = \left\{-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)+V(x,y)\right\}\psi(x,y) \tag{5}$$

Using Taylor Expansions this can be approximated to second order in Δ (the spatial grid spacing) by

$$H\psi^t_{x,y} = -\frac{\hbar^2}{2m\Delta^2}\left(\psi^t_{x+1,y}+\psi^t_{x-1,y}+\psi^t_{x,y+1}+\psi^t_{x,y-1}-4\psi^t_{x,y}\right)+V_{x,y}\psi^t_{x,y} \tag{6}$$

Where once again the x and y indices refer to the discrete space. Substituting this in Eqn (4) above, re-ordering and defining various other terms then gives

$$\zeta_{x,y}\psi^{t+1}_{x,y}+\psi^{t+1}_{x+1,y}+\psi^{t+1}_{x-1,y}+\psi^{t+1}_{x,y+1}+\psi^{t+1}_{x,y-1} = \Omega^t_{x,y} \tag{7}$$

where

$$\zeta_{x,y} \equiv i\beta - 4 - \gamma V_{x,y} \tag{8a}$$

$$\beta \equiv \frac{4m\Delta^2}{\hbar\Delta t} \tag{8b}$$

$$\gamma \equiv \frac{2m\Delta^2}{\hbar^2} \tag{8c}$$

$$\Omega^t_{x,y} \equiv \left(4+\gamma V_{x,y}+i\beta\right)\psi^t_{x,y}-\psi^t_{x+1,y}-\psi^t_{x-1,y}-\psi^t_{x,y+1}-\psi^t_{x,y-1} \tag{8d}$$

The algorithm we use to solve this set of equations is Chebyshev Accelerated Simultaneous Over Relaxation, a succesive approximation method. The residual is defined as

$$\xi^{i+1}_{x,y} \equiv \zeta_{x,y}\psi^i_{x,y}+\psi^i_{x+1,y}+\psi^i_{x-1,y}+\psi^i_{x,y+1}+\psi^i_{x,y-1}-\Omega^t_{x,y} \tag{9}$$

where the i index refers to each iteration. This is iterated repeatedly in a chessboard fashion (i.e. odd/even) using

$$\psi^{i+1}_{x,y} = \psi^i_{x,y} - \frac{\omega\xi^{i+1}_{x,y}}{\zeta_{x,y}} \tag{10}$$

until the residual is sufficently small. The initial wave function for each set of iterations is taken as that for the previous time step. ω is defined by

$$\omega^0 = 1$$

$$\omega^1 = \frac{1}{(1-\frac{1}{2}\rho_J^2)} \tag{11}$$

$$\omega^{n+1} = \frac{1}{(1-\frac{1}{4}\rho_J^2\omega^n)}$$

where ρ_J is the spectral radius of the Jacobian method i.e.

$$\rho_J = \tfrac{1}{2}(\cos(\pi/J) + \cos(\pi/L)) \tag{12}$$

and J and L are the number of grid points in each direction.

IV. Inclusion of a magnetic field

The basics of this algorithm remain the same when magnetic field is included and when it is adapted for two 1D interacting electrons.Using the symmetric gauge Eqns (7) & (8) become

$$\zeta_{x,y}\psi^{t+1}_{x,y} + (1-i\theta y)\psi^{t+1}_{x+1,y} + (1+i\theta y)\psi^{t+1}_{x-1,y} + (1-i\theta x)\psi^{t+1}_{x,y+1} + (1+i\theta x)\psi^{t+1}_{x,y-1} = \Omega^t_{x,y} \tag{7a}$$

where

$$\zeta_{x,y} \equiv i\beta - 4 - \gamma W_{x,y} - \phi(x^2+y^2) \tag{8a}$$

$$\beta \equiv \frac{4m\Delta^2}{\hbar\Delta t} \tag{8b}$$

$$\gamma \equiv \frac{2m\Delta^2}{\hbar^2} \tag{8c}$$

$$\Omega^t_{x,y} \equiv \left(4 + \gamma W_{x,y} + i\beta + \phi(x^2+y^2)\right)\psi^t_{x,y} - (1-i\theta y)\psi^t_{x+1,y} \tag{8d}$$
$$-(1+i\theta y)\psi^t_{x-1,y} - (1-i\theta x)\psi^t_{x,y+1} - (1+i\theta x)\psi^t_{x,y-1}$$

$$\theta = meB\Delta^2 \tag{8e}$$

$$\phi = \frac{me^2B^2\Delta^4}{2\hbar} \tag{8f}$$

The residual is then defined by

$$\xi^{i+1}_{x,y} \equiv \zeta_{x,y}\psi^i_{x,y} + (1-i\theta y)\psi^{t+1}_{x+1,y} + (1+i\theta y)\psi^{t+1}_{x-1,y} + (1-i\theta x)\psi^{t+1}_{x,y+1} \tag{9a}$$
$$+(1+i\theta x)\psi^{t+1}_{x,y-1} - \Omega^t_{x,y}$$

and used as before to solve for each succesive approximation.

V. Two Electron case

If we consider x and y as the 1D coordinates of two interacting electrons the time independent Schrödinger equation can be written identically to Eqn (5) above with

$$V(x,y) = \frac{e^2}{4\pi\varepsilon_0|x-y|} + V_1(x) + V_1(y) \tag{13}$$

where V_1 is the 1D electrostatic confinement potential.Therefore using this as the potential enables us to use identical methods as above.

VI. Parallelisation

The 2 dimensional grid is split evenly over a rectangular array of transputers which iterate their own section of grid and swap boundary conditions at each time step.

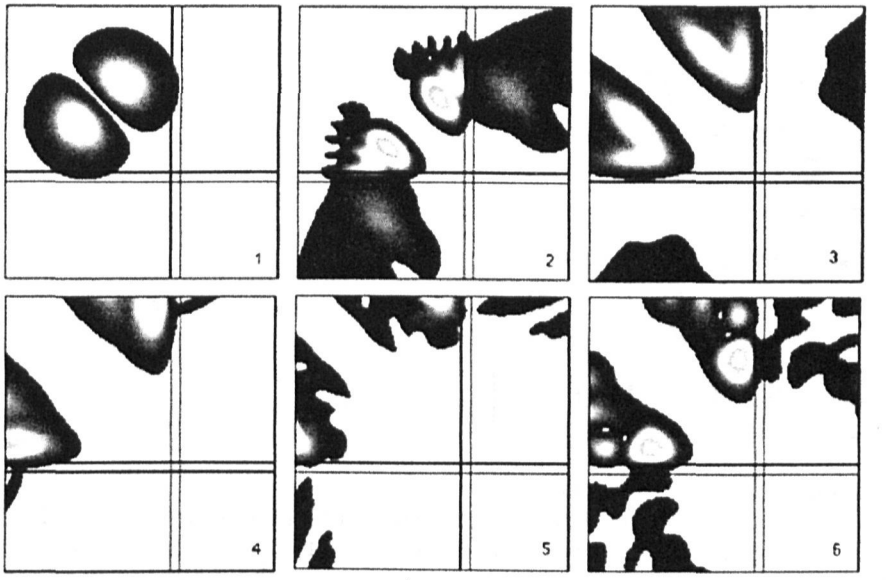

Figure 2(a) Contour plot of modulus of 2-electron wavefunction in configuration space

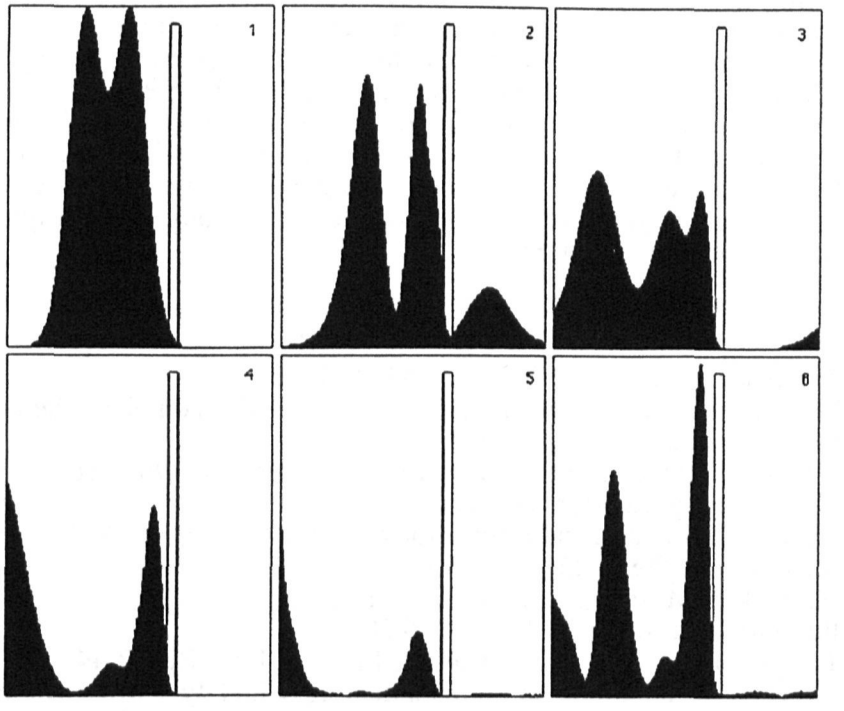

Figure 2(b) Projected total charge distribution in direct space for time sequence of Fig 2a.

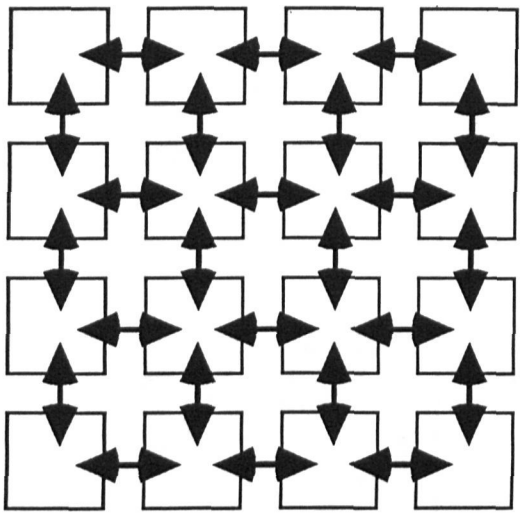

Figure (1) transputer linkage (4 x 4 case)
The method is parallelised on a 64 transputer array and runs at approximately 200 MFLOPS. The results of this study are also being used to validate a novel algorithm for *few electron* transport in *2 dimensions* based upon an extension of the *coupled-mode formalism* [8] developed for 1 electron 2D tranport. Applications to chaos in magnetic fields are in progress.

VII. Coulomb assisted resonant tunnelling in quasi-1D electron systems.

For the case of 2-interacting electrons transporting/tunneling through bottlenecks in small arrays of quantum point contacts we have identified a new resonant tunnelling process which arises from the tunnelling decay from the quasi-confinement of one electron between a second following electron and a downstream potential barrier. The effect requires mono-mode conduction. Hitherto, only the combination of conventional resonant tunnelling with Coulomb blockade from the charging of the intermediate quantum well has been identified. Figure (2) shows the case of two equal spin electrons initially 30 nm apart (Coulomb energy 4.5 meV) encountering a barrier of height 50 meV , width 5 nm for incident kinetic energy of 10 meV/electron for electrons in GaAs. The effect is strongly damped unless the electron stream is strongly correlated in space and time. Coupled quantum dots, long chain polymers, enzymes, redox chains provide possible test cases.

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