P-16

Numerical simulation of a two-particle wave function in quantum wires

S. Reggiani, A. Bertoni, M. Rudan
Advanced Research Center for Electronic Systems (ARCES)
Dept. of Electronics, Univ. of Bologna, Viale Risorgimento, 2, 40136 Bologna, Italy
Tel.+39 051 2093773, Fax. +39 051 2093779
e-mail: sreggiani@deis.unibo.it

Abstract— As the key requirement of a quantum computer is the creation and exploitation of entanglement, a detailed study of entangled states has been carried out with reference to a solid-state system based on coupled quantum wires. A brief review of the basic gates is given first, based on preliminary investigations, followed by the analysis of electrons running along coupled quantum wires. The particle dynamics has numerically been simulated by means of a time-dependent Schrödinger solver applied to a two-particle system. Results are reported showing entangled states created by means of suitable quantum-gate networks. Starting from these fundamental results, the complexity of some interesting circuits is addressed, showing both the application of the universal set of quantum gates to complex algorithms and the computational speed-up achieved within the proposed implementation.

I. INTRODUCTION

In the present work we aim at investigating the solid-state implementation of quantum networks based on coherent electron transport in coupled quantum wires. In a previous work [1] the charge state of an electron running along two quantum wires has been adopted for the definition of qubit. Subsequently, the design of one- and two-qubit gates has been addressed in order to define the universal set of quantum gates and, following [2], a basic set of three (two single-qubit and one two-qubit) transformations has been analyzed and simulated [3], [4]. More specifically, a single-qubit gate that realizes a wave packet splitter $\mathbf{S}_x$ has been designed by introducing a coupling window between the wires, that enables a tunneling process of the wave packet; the second single-qubit gate that realizes a phase shifter, $\mathbf{R}_0$ or $\mathbf{R}_1$, is given by the application of a potential barrier able to delay the propagation of an electron along one of the two wires (with label 0, or 1, respectively). Finally, the two-qubit gate is constituted by a Coulomb coupler $\mathbf{T}$, i.e., a region where the wires belonging to adjacent qubits get close enough to determine a mutual interaction. The proposed physical system can be realized using intrinsic GaAs within a GaAs-$Al_xGa_{1-x}As$ heterostructure or, alternatively, silicon fully surrounded by SiO_2. The qubit states $|0\rangle$ and $|1\rangle$ are represented by the localization of the electron wave function in one of the two wires: the states are, respectively, the sum and difference of the two lower eigenfunctions of the coupled wires potential with respect to the quantized direction orthogonal to the wires (double-well structure). The electron coherently propagates along the longitudinal direction. Such a system is within the reach of the mesoscopic semiconductors technology [5].

II. NUMERICAL SIMULATION OF ENTANGLEMENT

In the previous works, the proposed system was designed and tested by solving the 2D time-dependent Schrödinger equation for single electrons with mutual Coulombic interaction. Such architecture of the quantum devices for the realization of the universal set has been validated using a base of factorizable qubit states. Within this approach, no entanglement between electrons can numerically be simulated. In order to overcome this limitation, a novel two-particle approach has been used. In this work, the dynamics of the electrons running along the wires has been solved by applying the Schrödinger equation to the whole two-particle wave function. To this purpose, the wires have been modeled as 1D devices so that the spatial domain is only given by the product of the wire lengths, this reducing the computational effort. The pattern of the quantum wires has actually been taken into account in the calculation of the electron-electron interaction as the electron distance, which gives its contribution in the Coulomb potential, as explained in the following.

A. THEORETICAL ASPECTS

From a theoretical point of view, the effect of entangled states can easily be deduced once the behavior of the system on a given basis set is known, thanks to the superposition principle. In order to study non-separable (i.e., entangled) states by means of a numerical simulation, the time-dependent Schrödinger equation for the full two-particle wave function $\psi(x_1, y_1, x_2, y_2, t)$ must be solved. Such approach is rather expensive from a computational point of view. To overcome this difficulty a reduction of the dimensionality is required: a semi-1D model for the quantum-wire structures has been used to realize the numerical solver. Within the semi-1D domain, the variables x_1 and x_2 take only the 0 or 1 values to indicate the wires where the electrons are localized, leading to the wave function $\psi_{x_1,x_2}(y_1, y_2, t)$. The latter is constituted by four different components corresponding to the four configurations of the x_1 and x_2 variables. The coherent transport of the two electrons running along the structure made of two qubits (i.e., four wires) has been simulated by solving the following equation for the four

different components of the wave function:

$$i\hbar\frac{\partial}{\partial t}\psi_{x_1,x_2}(y_1,y_2,t) = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial y_1^2}+\frac{\partial^2}{\partial y_2^2}\right)\psi_{x_1,x_2}(y_1,y_2,t) + +V_{x_1,x_2}(y_1,y_2)\psi_{x_1,x_2}(y_1,y_2,t) \quad (1)$$

where $V_{x_1,x_2}(y_1,y_2)$ is the electric potential experienced by the two particles and m the effective mass in the spherical-parabolic approximation. More specifically, the geometry of the system is contained in the two-particle potential $V_{x_1,x_2}(y_1,y_2)$, which consists of three terms: the two potentials along the wires 0 and 1 of each qubit (U), due to the device structure, and the Coulombic interaction between the electrons:

$$V_{x_1,x_2}(y_1,y_2) = U_{x_1}(y_1)+U_{x_2}(y_2)+\frac{e^2/(4\pi\epsilon)}{D_{x_1,x_2}(y_1,y_2)}, \quad (2)$$

where $D_{x_1,x_2}(y_1,y_2)$ is the distance between point y_1 in the x_1 wire of the first qubit, and point y_2 in the x_2 wire of the second qubit:

$$D_{x_1,x_2}(y_1,y_2) = \sqrt{[p_{x_1}(y_1)-p_{x_2}(y_2)]^2+[y_1-y_2]^2}, \quad (3)$$

where $p_{x_i}(y_i)$ gives the x coordinate of the x_i wire corresponding to the y_i position along the wire.

Let us consider the 1D application of the three fundamental gates mentioned above. As far as the wave packet splitter is concerned, it is not possible to simulate directly the wave-function splitting induced by a coupling window, as the splitting comes from the transverse dynamics whose description is lost. On the other hand, the electron splitter $\mathbf{S}_x$ is a single-qubit transformation and no entanglement is involved. Moreover, the numerical simulations of the gate by a 2D Schrödinger solver [4] show that, after the $\mathbf{S}_x$ transformation, the transversal component of the electron wave function is still described, in each wire, by the ground state of an infinite square well taken as the transverse initial condition. Thus, along the whole device, except for the regions of the coupling windows, the transversal dynamics can be neglected. The above considerations allow one to include the effect of the $\mathbf{S}_x(\theta)$ gate in the frame of the semi-1D model by means of the application of its corresponding matrix, like a "black-box" function. The phase shifter $\mathbf{R}_0$ ($\mathbf{R}_1$) is obtained with a delaying potential barrier inserted along a wire and incorporated in the potential function $U_0(y_i)$ ($U_1(y_i)$). Finally, the conditional phase shifter $\mathbf{T}$ is, among the three considered here, the only two-qubit gate and, as a consequence, the only one able to produce an entangled state. It is simulated by introducing the description of the geometrical shape of the wires along the transversal direction using the $p_{x_i}(y_i)$ functions. To study the optimal geometry for the quantum-wire system, able to perform the $\mathbf{T}(\gamma)$ transformation, a number of simulations have been performed varying two geometric parameters: the length of the Coulomb coupler and the distance between the coupled wires [6].

B. SIMULATION RESULTS

The simulations have been performed for a Si-SiO_2 system, with a distance between the coupled wires of 10 nm and a distance between the two qubit systems of 60 nm. The electrons are injected in the $x_i = 0$ wires; the initial wave packet is given by the product of two minimum-uncertainty Gaussian functions with a standard deviation $\sigma = 18$ nm and a momentum k corresponding to a 20 meV energy. Two different networks have been simulated. The first one is shown in Fig. 1. The network is

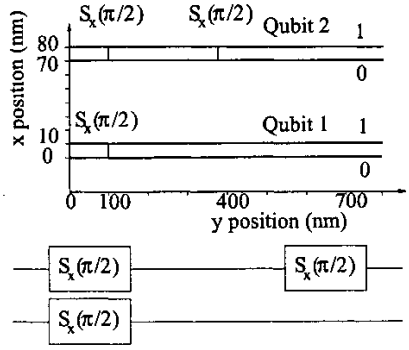

Figure 1. Architectural scheme and quantum circuit of the first network: $\mathbf{S}_x$ represents the coupling-window gate that realizes the wave-packet splitter.

constituted by three wave-packet splitters $\mathbf{S}_x(\pi/2)$. The corresponding matrix reads:

$$\mathbf{S}_x(\pi/2) = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix}. \quad (4)$$

By applying the first two gates to the initial state $|00\rangle$, one obtains the superposition of states:

$$\frac{1}{2}\left(|00\rangle + i|01\rangle + i|10\rangle - |11\rangle\right). \quad (5)$$

Then the wavepacket experiences the third gate applied to the second qubit, leading to the final state:

$$\frac{1}{\sqrt{2}}\left(i|01\rangle - |11\rangle\right) = \frac{1}{\sqrt{2}}\left(i|0\rangle - |1\rangle\right)|1\rangle, \quad (6)$$

showing that the final state of the two-qubit system is non-entangled. In Fig. 2 the numerical simulation confirms the result of (6), showing the propagation of the two-particle wave packet over the four configurations.

The second network (Fig. 3) is similar to the previous one, except for the gate $\mathbf{T}(\pi/2)$ realized before the third splitter.In this case, the creation of an entangled final state is achieved. The two-qubit transformation induced by the $\mathbf{T}(\pi/2)$ gate is:

$$\mathbf{T}(\pi/2) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & i & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \quad (7)$$

The application of $\mathbf{T}$ to the superposition of states created by the first two splitters (Eq. 5) gives the final entangled state:

$$\frac{1}{2\sqrt{2}}\left[2i|01\rangle - (i+1)\left(|10\rangle + |11\rangle\right)\right]. \quad (8)$$

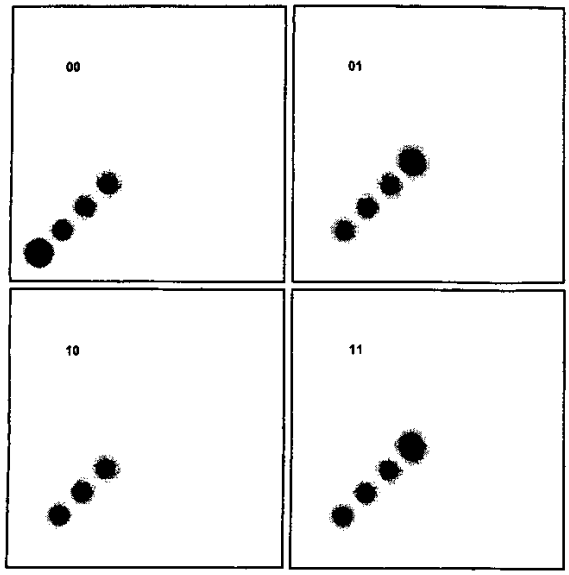

Figure 2. Square modulus of the two-particle wave function at different time steps for the network of Fig. 1. The four graphs represent the $Y_1 \times Y_2$ domain of the wave function (800 nm × 800 nm). Each graph corresponds to a possible wire configuration. The initial condition $|00\rangle$ at time 0 is given by the wave packet shown in the lower-left corner of the 00 graph. The time step used for this representation is 500 fs.

In Fig. 4, the numerical results for the second network are reported with the same initial condition and time step as in Fig. 2. The numerical integration of the final electronic density for each configuration has been carried out in order to compare the numerical result with the analytical one. It is found that the wave-packet splitting is: 25% in both the $|10\rangle$ and $|11\rangle$ states, 37% in the $|01\rangle$ state, and 13% in the $|00\rangle$ state. This is in contrast with equation (8), which predicts a 25%, 25%, 50%, and 0% splitting. The unexpected 13% is due to the deformation effect of the Coulomb coupler, which causes an undesired spreading of the wave function in the 10 wire configuration.

III. COMPLEXITY OF QUANTUM NETWORKS

As reported above, a number of runs have been carried out on simple quantum networks. We have also investigated more complex algorithms from an architectural point of view. More specifically, the complexity of the quantum networks has been analyzed by taking into account the main delays affecting the computation, given by the application of the two-qubit Coulomb coupler $\mathbf{T}(\phi)$ or, equally, the controlled-NOT gate. As a first fundamental network, the controlled-controlled-NOT (CCNOT) gate [7], which realizes the Toffoli gate, has been addressed. The CCNOT gate negates the target qubit if and only if the AND of the two control qubits is 1.

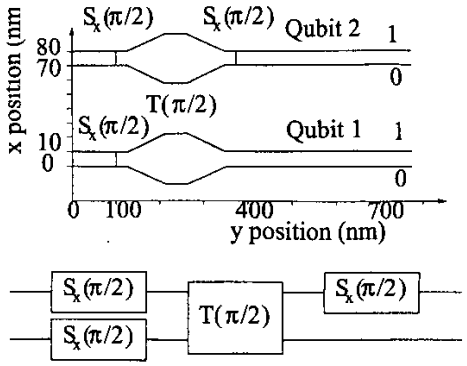

Figure 3. Architectural scheme and quantum circuit of the second network. **T** represents the Coulomb coupler, formed where the inner wires get close enough to give rise to a mutual interaction.

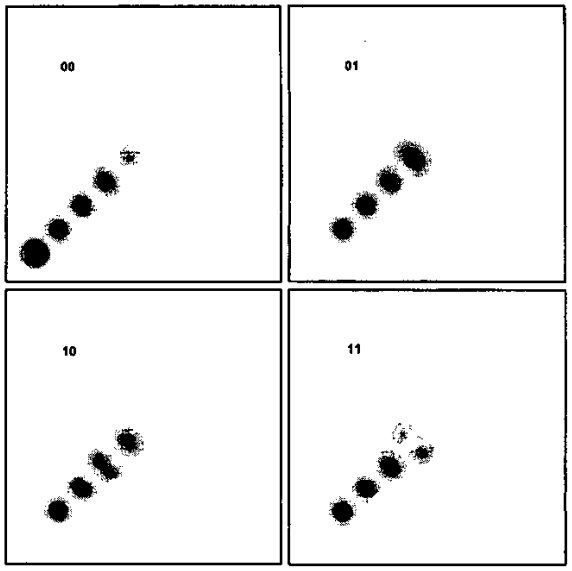

Figure 4. Square modulus of the two-particle wave function at different time steps for the network of Fig. 3. The deformation effect of the **T** gate becomes relevant at $t = 1500$ fs.

In Fig. 5, the CCNOT network is shown along with the adopted symbols. As a second example, a quantum full adder is shown in Fig. 6. It worth noting that, since the physical system allows for the application of basic gates only to adjacent qubits, one or more exchange gates must be suitably placed each time non-adjacent qubits are involved in a transformation. This contributes to the network complexity. In the proposed implementation the exchange gate, that swaps the quantum information of two adjacent qubits in order to consequently change their position, is constituted by the cascade of three controlled-NOT gates. By taking into account only the main delays affecting the computation, given by the application of the two-qubit elementary gates, the complexity of the

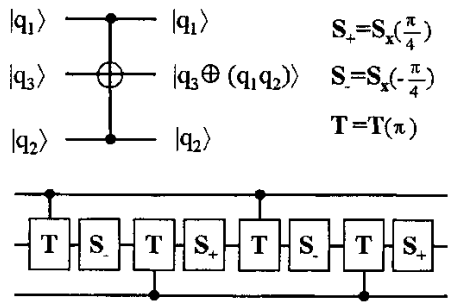

Figure 5. Quantum network for the controlled-controlled-NOT gate.

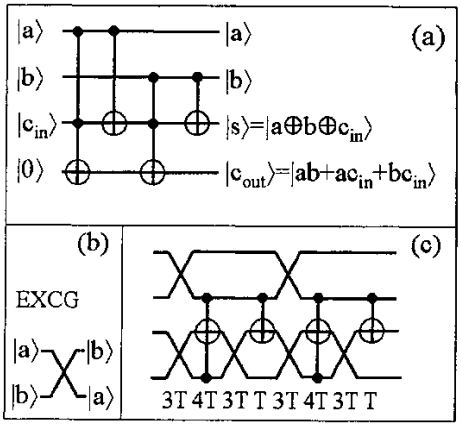

Figure 6. (a) Logic network for the quantum full adder. (b) Symbol adopted for the exchange gate. (c) Architectural scheme for the quantum full adder. The bottom line indicates the number of **T** gates for each step.

quantum full adder corresponds to 22 gates. The analysis of a quantum network that realizes the quantum fast Fourier transform (QDFT) has already been carried out in the literature as a first important example of quantum algorithm [8]. Within the adopted physical system, a straightforward realization of the network has been obtained. The architectural scheme of the QDFT network is shown in Fig. 7. It is worth noting that the final bit-reversed configuration, which characterizes the usual fast Fourier transform algorithm, has been avoided by means of the applied exchange gates. Starting from the analysis of a 4-qubit structure, it is easy to generalize the network to L qubits, obtaining a complexity corresponding to $4 \times (2L-3)$ gates. The exponential speed-up that can be achieved in terms of computational time by applying the quantum DFT circuit is obtained by exploiting the massive quantum parallelism in the preparation of the initial state: in this way, one can calculate the DFT applied to a superposition of states instead of a single state, and simultaneously calculate the whole set of coefficients. This transformation is applied to most of the quantum algorithms shown in the literature [7].

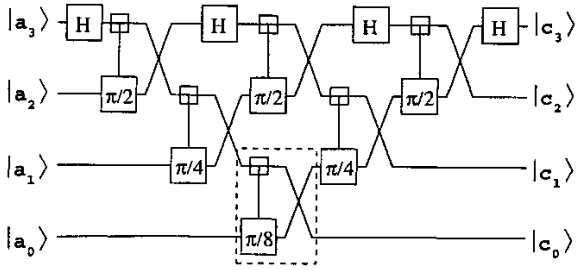

Figure 7. Quantum discrete Fourier transform: schematic network for a 4-qubit QDFT. The **H** gate is a Hadamard transformation [2],the controlled gate is a conditional phase shifter whose angle is indicated by the label, the EXCG gate is used to suitably swap the qubit positions. $|A\rangle$ is the input state of the L-qubit register, and $|C\rangle$ is the set of states of the final superposition that constitutes the DFT coefficients.

IV. ACKNOWLEDGEMENTS

This work has partially been supported by the Italian Ministry of Education, University and Research MIUR under the National Project on Quantum Computation, and by the U. S. Office of Naval Research (Contract n. N00014-98-1-0777).

REFERENCES

[1] A. Bertoni, P. Bordone, R. Brunetti, C. Jacoboni, S. Reggiani, "Quantum logic gates based on coherent electron transport in quantum wires", *Phys. Rev. Lett. 84*, 5912 (2000); see also R. Ionicioiu, G. Amaratunga, F. Udrea, *Int. J. Mod. Phys. B15*, 125 (2001) - quant-ph/9907043.

[2] A. Barenco, C. H. Bennett, R. Cleve, D. P. DiVincenzo, N. Margolus, P. Shor, T. Sleator, J. A. Smolin, H. Weinfurter, *Phys. Rev. A 52*, 3457 (1995).

[3] S. Reggiani, A. Bertoni, P. Bordone, R. Brunetti, C. Jacoboni, M. Rudan, G. Baccarani, "Two-qubit gates based on coupled quantum wires", *Proc. SISPAD 2000*, IEEE Cat. N. 00TH8502, 184 (2000).

[4] A. Bertoni, P. Bordone, R. Brunetti, C. Jacoboni, S. Reggiani, accepted for publication in *J. Mod. Opt.* (2002).

[5] Y. Nakajima, Y. Takahashi, S. Horiguchi, K. Iwadate, H. Namatsu, K. Kurihara and M. Tabe, "Quantized conductance of a silicon wire fabricated by separation-by-implanted-oxygen technology", *Jpn. J. Appl. Phys. 34*, 1309 (1995).

[6] A. Bertoni, R. Ionicioiu, P. Zanardi, F. Rossi, C. Jacoboni, *Physica B*, in press. S. Reggiani, A. Bertoni, M. Rudan *Physica B*, in press.

[7] D. Deutsch, *Proc. R. Soc. London Ser. A 425*, 73 (1989). P. W. Shor, *Proc. of the 35th Annual Simposium on the Foundations of Computer Science (IEEE Comp. Sci. Soc.)*, 166 (1994). A. Ekert and R. Jozsa, *Rev. Mod. Phys. 68*, 733 (1996).

[8] D. Coppersmith, *IBM Research Report RC 19642* (1994) - quant-ph/0201067.