Electron Emission From a Quantum Well as a Result of Exchange and Coulomb Interactions

M. Cahay and T. Singh
Device Simulation Laboratory
Department of Electrical and Computer Engineering
University of Cincinnati, Cincinnati OH 45221

S. Bandyopadhyay
Department of Electrical Engineering
University of Notre Dame
Notre Dame, Indiana 46556

Abstract

The role of Coulomb and exchange interactions on the dynamics of two-electron systems in semiconductor nanostructures has received widespread attention over the last few years [1-7]. In this paper, we study the time evolution of a two-electron wavepacket in a finite quantum wire whose potential profile consists of three identical wells evenly spaced. Initially, both electrons are placed in the lowest bound state of the structure and both are localized mainly in the middle well. However, as a result of Coulomb and exchange interactions, the two electrons gradually move to higher boundstates to finally relocate themselves in the left and right wells. The typical time scale for this process to occur is within the subpicosecond regime. The time evolution of the two-particle wavefunction is examined by numerically solving the two-particle time-dependent Schrödinger equation using the Alternating Direction Implicit Algorithm [8-9].

1 Introduction

Recently, a number of researchers have studied the role of electron-electron interaction in semiconductor nanostructures in which energy quantization of the electrons cannot be neglected [4-11]. Phenomena that lend themselves to this regime include "Coulomb Exclusion" as opposed to its semiclassical counterpart "Coulomb Blockade", the effects of exchange and correlation on the tunneling probability of an electron through a nanostructure in the presence of an occupied boundstate in the structure [5,6], many-body effects influencing the quantum lifetime of quasi-particle in a quantum wire [7], etc. It was also shown the electron-electron interaction effects for spin-parallel and spin-antiparallel electrons lead to specific peaks in the transmission probability through laterally confined resonant tunneling devices [10]. More recently, Buttiker has discussed the possibility of observing flux sensitive interference effects between mutually incoherent quantum channels as a result of exchange interaction [11].

In this paper, we complement those studies by investigating the dynamics of a two-electron system in the triple-well configuration as shown in figure 1. In the past, the probability density of the groundstate two-particle wavefunction for a system of two electrons in a two-well configuration separated by a small barrier was calculated [4]. The energy of this boundstate was recalculated for various applied bias across the two wells. In contrast, our simulations deal with the time-evolution of an initial two-particle wavefunction for which the total energy of the two-particle is fixed. This allows us to investigate the effect of the Coulomb and exchange interactions on the dynamics of the two-particle system, i.e, on the redistribution of the total energy between its two-particle and one-particle contributions as the time evolves.

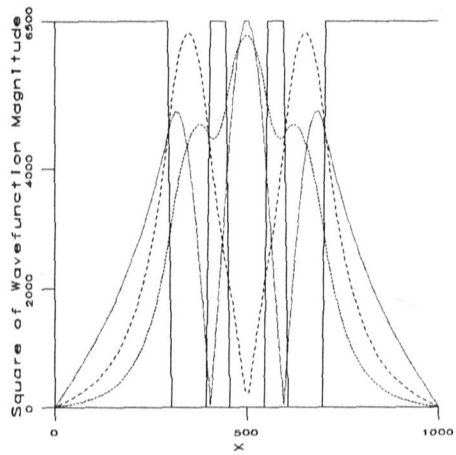

Figure 1: *Triple well configuration in a 1000 Å wide simulation domain. The three wells are identical (20 meV deep and 100 Å wide). The small dashed, long dashed, and dot-dashed lines show the one particle boundstates calculated using the program SEQUAL [13]. The effective mass is assumed to be $0.067m_0$ everywhere.*

2 Simulations

Our simulations were performed using the Alternating Direction Implicit Algorithm described in refs [8,9] to solve the two-particle Schrödinger equation:

$$i\hbar\frac{\partial}{\partial t}\Psi(x_1,x_2) = \left[-\frac{\hbar^2}{2m^*}\left(\frac{\partial^2}{\partial x_1^2}+\frac{\partial^2}{\partial x_2^2}\right) + E_c(x_1) + E_c(x_2) + V(|x_1-x_2|)\right]\Psi(x_1,x_2) \qquad (1)$$

where $E_c(x)$ is the conduction band potential energy profile and $V(|x_1-x_2|)$ is the Coulombic interaction potential between the two electrons. Because of the singular nature of the Coulombic interaction in one dimension, we replace the real Coulombic interaction with the regularized Coulomb potential derived by Banyai et al. [11],

$$V_{eff} = \frac{e^2}{4\pi\epsilon}\frac{1}{|x_1-x_2|+\delta}. \qquad (2)$$

This interaction approximates fairly well the interaction between two electrons in a quantum wire when δ is about one-third of the radius of the wire. The initial wavepacket describing the system of two electrons was chosen as the singlet state,

$$\Psi^S(x_1,x_2) = \Phi_1(x_1)\Phi_2(x_2) + \Phi_1(x_2)\Phi_2(x_1) \qquad (3)$$

with the two electrons located in the lowest boundstate of the three-well configuration shown in figure 1.

The latter consists of a system of three quantum wells, each being 100 Å wide and 20 meV deep. The separation between wells is fixed at 50 Å. The one-particle wavefunction for the triple-well configuration were calculated using the program SEQUAL [13] and are shown as dashed lines in figure 1. Choosing the top of the well as the reference energy level, the boundstate energy levels are given by -12.56, -8.37, and -1.90 meV. Figure 2 compares the 3-D plots of the probability densities $|\Psi(x_1,x_2))|^2$ after 0.01 ps, 0.1 ps, and 0.2 ps for the parameter δ in the regularized Coulomb potential equal to 333Å and 33Å, respectively.

A reduction in δ leads to a bigger repulsion between electrons. This variation in δ could be achieved experimentally through depletion of the quantum wire by a surrounding gate. Since the total energy of the two particles must be conserved, part of the Coulombic energy can be reduced if both electrons move to higher energy states of the triple-well configuration. This is clearly shown in right frames of figure 2.

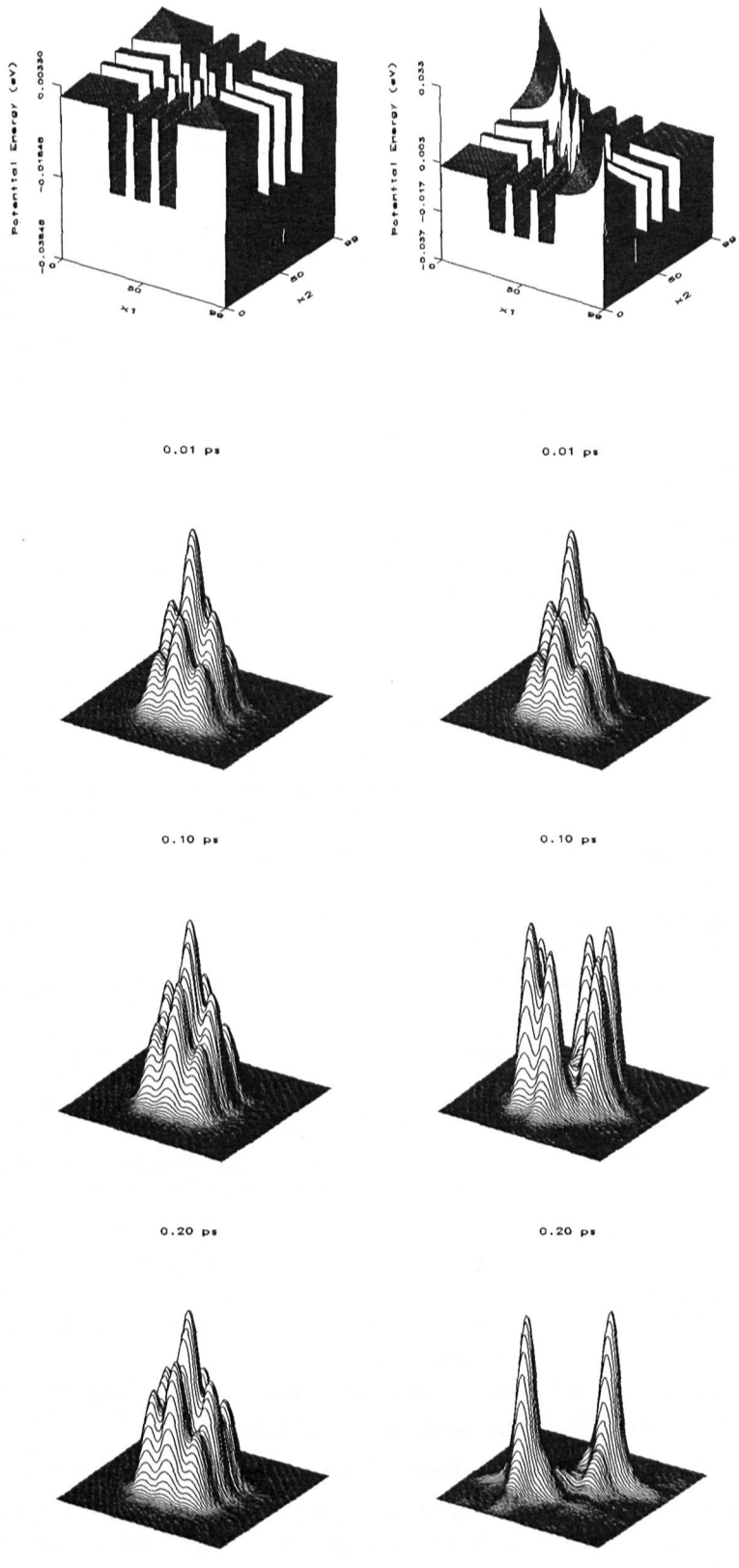

Figure 2: *Left frames: 3-D plots of the time evolution of the probability density of an initial two-electron wavepacket (eq.(3)) with both electrons in the lowest energy state wavefunction shown in figure 1. The parameter δ is equal to 333 Å. Right frames: Time evolution of the probability density with δ=33Å. The two upper frames show the total potential energy in eq.(1) for the case of δ=333Å (left), and δ=33Å (right), respectively. In this simulation $m^* = 0.067m_0$, ϵ=13.1ϵ_0, and 100 gridpoints were used in both directions.*

In the latter, we see that the Coulombic repulsion between electrons is strong enough to lead to electron transfer to the upper boundstates.

Notice also that the probability for both electrons to be located in the middle well is drastically reduced as the two electrons move to the side wells as a result of the Coulomb and Exchange interactions. This transfer is possible only if the parameter δ is small enough. Indeed, figure 2 indicates that not enough Coulombic potential energy is available for the case $\delta = 333\mathring{A}$. In this case, both electrons move only slightly apart from each other while remaining in the middle well. Experimentally, the two electrons could be excited in the middle well with a laser pulse and the switching to the side wells could be controlled with the use of a side gate surrounding the quantum wire.

Acknowledgment

M.C and T.S are supported by the National Science Foundation (Division of Electrical and Communications Systems) under Award N0. ECS-9108932. M.C and T.S acknowledge the Ohio Supercomputing Center for the use of their facilities. The work at Notre Dame was supported by the Air Force Office of Scientific Research under grant N0. AFOSR-91-0211 and by the Office of Naval Research under contract number N00014-91-J-1505.

References

[1] Proc. of the International Symposium on Nanostructures and Mesoscopic Systems-Santa Fe, New Mexico, May 20-24, 1991; edited by Wiley P. Kirk and Mark A. Reed (Academic Press), 1992.

[2] For an excellent review on the problems of electron correlation and Coulomb Blockade, see chapter 6 of ref.[1], pp. 227-295.

[3] V. J. Goldman, Bo Su, and J. E. Cunningham, "Single-Electron Resonant Tunneling Through Quantum Dots", pp. 173-182 in ref.[1].

[4] C. S. Lent, "Simple Quantum Models of Coulomb Effects in Semiconductor Nanostructures", pp. 183-193 in ref.[1].

[5] L. F. Register and K. Hess, "A Two-particle Model of Electron-Electron Interactions in Quantum Structures", pp. 369-378 in ref.[1].

[6] L. F. Register, V. Ravaioli, and K. Hess, *Journal of Applied Physics*, vol.69, no.10, 1185 (1991).

[7] V. B. Campos, S. Das Sarma, and M. A. Stroscio, "Hot electron relaxation in GaAs quantum wires", talk E19-8 presented at the APS March meeting, Indianapolis, March 1992.

[8] M. Cahay, J. P. Kreskovsky, and H. L. Grubin, *Solid-State Electronics*, vol.32, no.12, pp.1185-1189, 1989.

[9] T. Singh and M. Cahay, "Time-Dependent Analysis of Electron Wave Directional Couplers", Proceedings of the SPIE Symposium on Compound Semiconductor Physics and Devices, Sommerset, New Jersey, March 1992, to be published.

[10] A. Nakano, R. K. Kalia, and P. Vashista, *Physical Review B*, Vol. 44, no.15, 8121 (1991).

[11] M. Buttiker, *Physical Review Letters*, vol.68, no.6, 843, 1992.

[12] L. Banyai, I. Galbraith, C. Ell, and H. Haug, *Physical Review B*, vol.36, pp.6099-6104, 1987.

[13] M. J. McLennan and S. Datta, SEQUAL 2.1 User's Manual, Purdue University, TR EE89-17 (1989).