QUANTUM THEORY OF ELECTRON TRANSPORT IN MESOSCOPIC SYSTEMS

Final Technical Report
by
Carlo Jacoboni, Antonio Abramo, Paolo Bordone
(June 1996)

United States Army
EUROPEAN RESEARCH OFFICE OF THE U.S. ARMY
London England

CONTRACT NUMBER: N68171-95-C-9057
Istituto Nazionale per la Fisica della Materia,
Genova, Italy

Approved for Public Release; distribution unlimited

REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. AGENCY USE ONLY (Leave blank)	2. REPORT DATE	3. REPORT TYPE AND DATES COVERED
	30 June 1996	FINAL May 1995 -- April 1996

4. TITLE AND SUBTITLE
Quantum theory of electron transport in mesoscopic systems

5. FUNDING NUMBERS
N68171-95-C-9057

6. AUTHOR(S)
Carlo Jacoboni, Antonio Abramo, Paolo Bordone

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
Istituto Nazionale per la Fisica della Materia
Via dell'Acciaio 139
I 16153 Genova
Italy

8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)
European Research Office
Army Research Office
Office of Naval Research

10. SPONSORING/MONITORING AGENCY REPORT NUMBER

11. SUPPLEMENTARY NOTES

12a. DISTRIBUTION/AVAILABILITY STATEMENT

12b. DISTRIBUTION CODE

13. ABSTRACT (Maximum 200 words)

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14. SUBJECT TERMS			15. NUMBER OF PAGES
			16. PRICE CODE
17. SECURITY CLASSIFICATION OF REPORT	18. SECURITY CLASSIFICATION OF THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT

Abstract

The purpose of the work done under this contract has been to develop a general approach to the analysis of quantum transport in mesoscopic structures, allowing the extension to the quantum case of the methodologies assessed in the field of semiclassical electron transport. This aim has been pursued in the frame of the Wigner function formalism. The main feature of the chosen approach is to include the potential profile in the unperturbed Hamiltonian, leaving to the perturbed one the scattering terms only. This goal has been already partially achieved in the one-dimensional case, while for the two-dimensional one, only the coherent (unperturbed) dynamics has been investigated so far. As for the one-dimansional case, the dynamics of a travelling wave packet subject to a single phonon scattering has been investigated. Furthermore, the iterative solution at first-order in the electron-phonon interaction of the resulting Wigner dynamics has been analyzed for an open-boundary one-dimensional system. Finally, coherent transport in open-boundary two-dimensional system has been widely investigated. In this report we will illustrate the principal theoretical achievements obtained during this contract period, together with the main application results.

keywords: quantum transport, Wigner function, mesoscopic systems.

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1. Introduction

Mesoscopic systems have been widely investigated in recent years. This increasing interest is mainly related to the fundamental physical problems involved in their description, as to possible future utilization of such structures in the electronic devices production. Being that mesoscopic dimensions are comparable to the typical electron coherent length, a correct analysis of transport phenomena in mesoscopic devices requires detailed quantum mechanical treatment.

To this purpose, the Wigner function is a suitable tool, since it provides a rigorous quantum mechanical approach, and constitutes the more direct link between quantum and the semi-classical descriptions of the phase-space evolution in terms of a distribution function $f(\boldsymbol{r},\boldsymbol{k},t)$.

The Wigner function is defined as the Weil-Wigner transform of the density operator:

$$f^{w}(K,z)=\frac{1}{2\pi}\int_{-\infty}^{+\infty}d\eta \quad e^{iK\eta} \quad \langle z-\tfrac{1}{2}\eta|\Psi\rangle\langle\Psi|z+\tfrac{1}{2}\eta\rangle$$

and it has several interesting properties. When integrated with respect to K or z, it gives the correct probability for the different values of the coordinates and momentua, respectively. Furthermore, one may get for the state Ψ the correct expectation values of any function of its coordinates or momenta.

In the following section, we will illustrate some theoretical details concerning the Wigner function approach as we applied it to our general problem.

2. Wigner function theory for electron-phonon interaction

In this section the developed theory of quantum electron transport based on the extension of the Wigner function including electron-phonon coupling will be briefly reviewed.

We used an interaction scheme, where the electron potential profile (band engineering plus external applied voltage) is included in the unperturbed dynamics.

Let us consider a three-dimensional system of independent electrons (with translational invariance along x and y directions), interacting with phonons. The unperturbed Hamiltonian $\mathbf{H_0}$ of the system is:

$$\mathbf{H_0}=\mathbf{H_e}+\mathbf{H_p}=\frac{\mathbf{p}^2}{2m}+\mathbf{V}(z)+\sum_q \mathbf{a}_q^{+}\mathbf{a}_q\,\hbar\omega_q$$

where **p** and m are the electron momentum and mass, respectively, V(z) is the electron potential profile (including the applied voltage), $\mathbf{a_q}$ and $\mathbf{a_q}^+$ are the annihilation and creation operators of the phonon mode **q** with frequency ω_q. $\mathbf{H_{e\text{-}p}}$ is the electron-phonon interaction:

$$\mathbf{H_{e\text{-}p}}=\sum_q i\hbar F(q)[\mathbf{a}_q e^{i\mathbf{qr}}-\mathbf{a}_q^{+}e^{-i\mathbf{qr}}]$$

where F(q) is a function that depends on the type of electron-phonon interaction. In our case polar optical phonons have been considered.

The present theoretical approach starts from the definition of the Wigner function, generalized to include phonons in the system, together with one electron:

$$f(\mathbf{r},\mathbf{p},n_q,n_q')=\frac{1}{h^3}\int d\mathbf{r}'e^{-i\mathbf{p}\mathbf{r}'/\hbar}\rho(\mathbf{r}+\mathbf{r}'/2,n_q;\mathbf{r}-\mathbf{r}'/2,n_q')$$

where ρ is the density matrix of the electron-phonon system.

If we consider the density-matrix operator in the interaction picture with respect to the unperturbed hamiltonian $\mathbf{H_o}$, its corresponding Wigner function $\tilde{f}$ satisfies the equation of motion

$$\frac{\partial}{\partial t}\tilde{f}(\mathbf{r},\mathbf{p},n_q,n_q',t)=\frac{1}{h^3}\int d\mathbf{r}'e^{-i\mathbf{p}\cdot\mathbf{r}'/h}\langle \mathbf{r}+\mathbf{r}'/2,\mathrm{n}_q|[\tilde{\mathcal{H}}(t),\tilde{\rho}(\mathrm{t})]|\mathbf{r}-\mathbf{r}'/2,n_q'\rangle$$

where $\tilde{\mathcal{H}}'=\tilde{H}_{e-p}/i\hbar$.

Analytical elaborations allow to obtain a Neumann series for the problem, whose zero and second order terms yield the ballistic evolution of the Wigner function and contributions corresponding to one phonon scattering, respectively. The solution of the resulting problem can be obtained, for a generic potential profile, only through a numerical procedure.

First, the Schrödinger equation is numerically solved to determine the system eigenbasis. Since we are dealing with a one-dimensional problem, this numerical step doesn't present relevant inherent difficulties. However, particular care has to be devoted to the mesh refinement, in order to recover the orthogonality of the eigenstates. Then, the numerical integration of the Wigner function is performed. However, an analycal extension of the integration procedure is required to insure the normalization conditions in the asymptotic space region. The choice of the system boundary condition is a crucial problem itself. It is in fact known that the boundary conditions can drastically alter the dynamical evolution of a system, driving its behavior from stability to instability. An original treatment of the integration over the boundary conditions has been developed. As in all boundary problems, initial and boundary conditions are mandatory: the inital condition requires the knowledge of the unknown function in any point of the space at $t=0$, while boundary conditions require, at any t, its knowledge over the boundaries. However, since the definition of the Wigner function is clearly non-local in space, a correlation between the Wigner function inside and outside the system boundaries (where it is not known) is inherent to the Wigner formalisms. This implies a specific treatement of the boundary integration, consisting in the integration back in time over the boundaries to get the proper Wigner function boundary values at each needed time (see Fig. 2.1.).

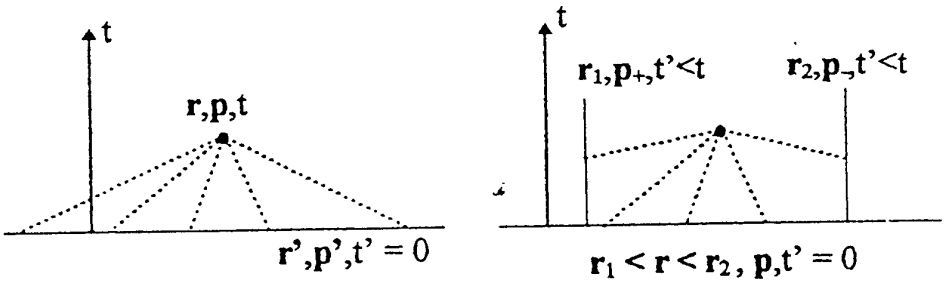

Fig. 2.1: Sketch of the boundary conditions treatment.

Results for the unperturbed Wigner function and for the perturbation corrections have been obtained for simple cases of interest.

As a side achievement, the study of the density of states in an open-boundary system has been carrier out. In this frame, the problem of the orthonormalization of scattering states with different limits for the potential term at $+\infty$ and $-\infty$ has been critically reviewed, and the fundamental relationship between the wave function normalization and the density of states has been clarified in the limit of a box of infinite length.

As implicitely stated above, the numerical difficulties related to the solution of the problem are very relevant. Therefore, a straightforward implementation of the algorithms is not satisfactory from the computational point of view. To this purpose, the analysis of the variance of the results has shown the necessity of *importance sampling* techniques to improve the computational efficiency of the numerical procedure. Such techniques are currently under development.

To provide a comparison with the quantum results, and a suitable hint to their interpretation, a semiclassical Monte Carlo code has been realized. To maintain as strong as possible the analogy with the quantum solution of the Wigner transport equation, the semiclassical code is based on the series expansion of the Boltzmann equation. In such a way it is possible to make a direct comparison between classical and quantum perturbative corrections to the distribution function (order by order). This procedure proves to be very succesfull in driving the quantum code development on the correct path, providing a quantitative insight on the quantum correction to expect.

To give an example of the obtained results, Fig. 2.2 shows the unperturbed (ballistic) Wigner function, as obtained from the scattering states entering a device with a Maxwellian distribution. The potential profile of the device is a ramp of uniform electric field.

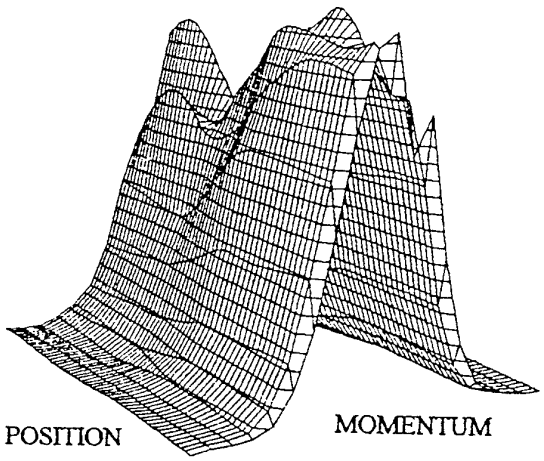

Fig. 2.2: Unperturbed Wigner function obtained with scattering states entering with a Maxwellian distribution a region with a potential ramp.

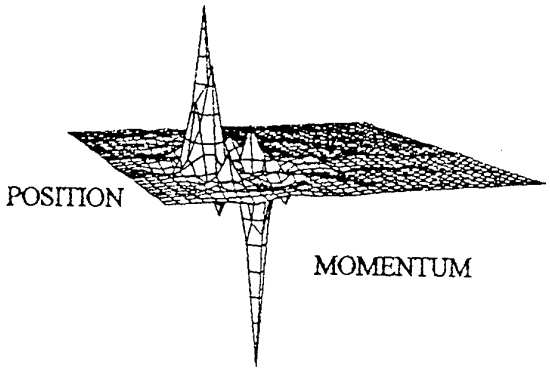

Fig. 2.3: Sample of second-order perturbation correction corresponding to a real and virtual phonon emission process.

Fig. 2.3 shows, for the case above, the second-order correction to the Wigner function due to a real and virtual eletron-phonon scattering process.

3. Wigner function of a step potential

From the anaytical side, the solution of the perturbed Wigner function has been derived for an open-boundary system in presence of an abrupt potential step. Since the system is open, the eigenstates above a certain energy are degenerate, and a proper linear combination of such eigenstates has to be chosen. It has been recognized that a natural basis is provided by the so called "scattering states". The proof of the degenerate scattering states orthonormality, very important for their use as a basis set, has been subject of discussion in the literature, and has been presented following a quite involved and indirect way. For the case of a step potential profile, we have derived such a proof in a straightforward way, performing the direct calculation on the scattering states, with the use of the formal expression

$$\int_{-\infty}^{+\infty} \theta(\pm x) e^{ikx} dx = \pi\delta(k) \pm iP\left(\frac{1}{k}\right)$$

where P means principal value and θ is the step function. The result shows that the scattering states are normalized to a δ–function.

One of the advantage of the Wigner function representation is that the mean value of any observable A is given, as in classical mechanics, by phase-space integrals with the Weil-Wigner transform of the corresponding operator

$$\langle A\rangle = \int dK \int dz A(K,z) f^{w}(K,z)$$

where

$$f^{w}(K,z) = \frac{1}{2\pi}\int e^{iK\eta}\,\rho(z-\eta/2, z+\eta/2)d\eta\,.$$

The Fourier transform included in the Wigner function definition imposes some requirements on the behavior of the density matrix ρ as a function of η. It can be shown that this Fourier transform can be justified if the eigenstates are normalized to unity. As stated before, scattering states are normalized to a δ-function, meaning that the required behavior for ρ can be provided only by the weight function g included in the density matrix definition for a mixture of states. Furthermore, we have shown that it is possible to define a Wigner function for pure states and to use it to evaluate an observable expectation value.

In fact, using an appropriate converging procedure, it is possible to write

$$f^{w}(K,z) = \int g(k') f_0^{w}(z,k',K)dk'$$

where

$$f_0^{w}(z,k',K) = \lim_{\alpha\to 0^+}\int e^{-\alpha|\eta|}e^{iK\eta}\,\rho_0(z,\eta)d\eta$$

is the pure state Wigner function, and α is a convergency factor.

In this frame, the observable expectation value is redifined in terms of a mixture of pure state expectation values, i.e.

$$\langle A\rangle = \int g(k)\int A(K) f_0^{w}(z,k',K)dKdk'.$$

4. Wave packet dynamics

The investigation has also faced the study of the dynamics of a wave packet subject to a single scattering process. A wave packet, obtained as a superposition of the system eigenstates, is studied while it undergoes a single phonon scattering process. Also in this case, the developed Wigner-function formalism has been used. As a case study, propagation through a resonant-tunneling double-barrier structure has been chosen.

A symmetrical double-barrier potential profile of height 0.2 eV has been considered, with barrier width of 20 Å and a well width of 100 Å. The eigenstates and the eigenvalues of the potential profile have been determined through the numerical solution of the associated Schrödinger equation.

The system is located in a "universe" infinite well of lenght 10^4 Å, which still allows to deal with normalized electron states, but is large enough not to influence the electron dynamics under investigation.

We have analyzed the influence on the unperturbed wave packet Wigner function of a single phonon back-scattering event. The unperturbed Wigner function is damped away to leave the perturbation term only. Fig. 4.1 shows the evolution of the unperturbed electron wave packet, where the probability density as a function of the z coordinate is reported.

The associated Wigner function is shown in Fig. 4.2. Notice how the wave packet peaks inside the quantum well after about 1ps and then how it smeares out.

Fig. 4.3 shows the evolution of the Wigner function of the scatterd wave packet during the scattering process.

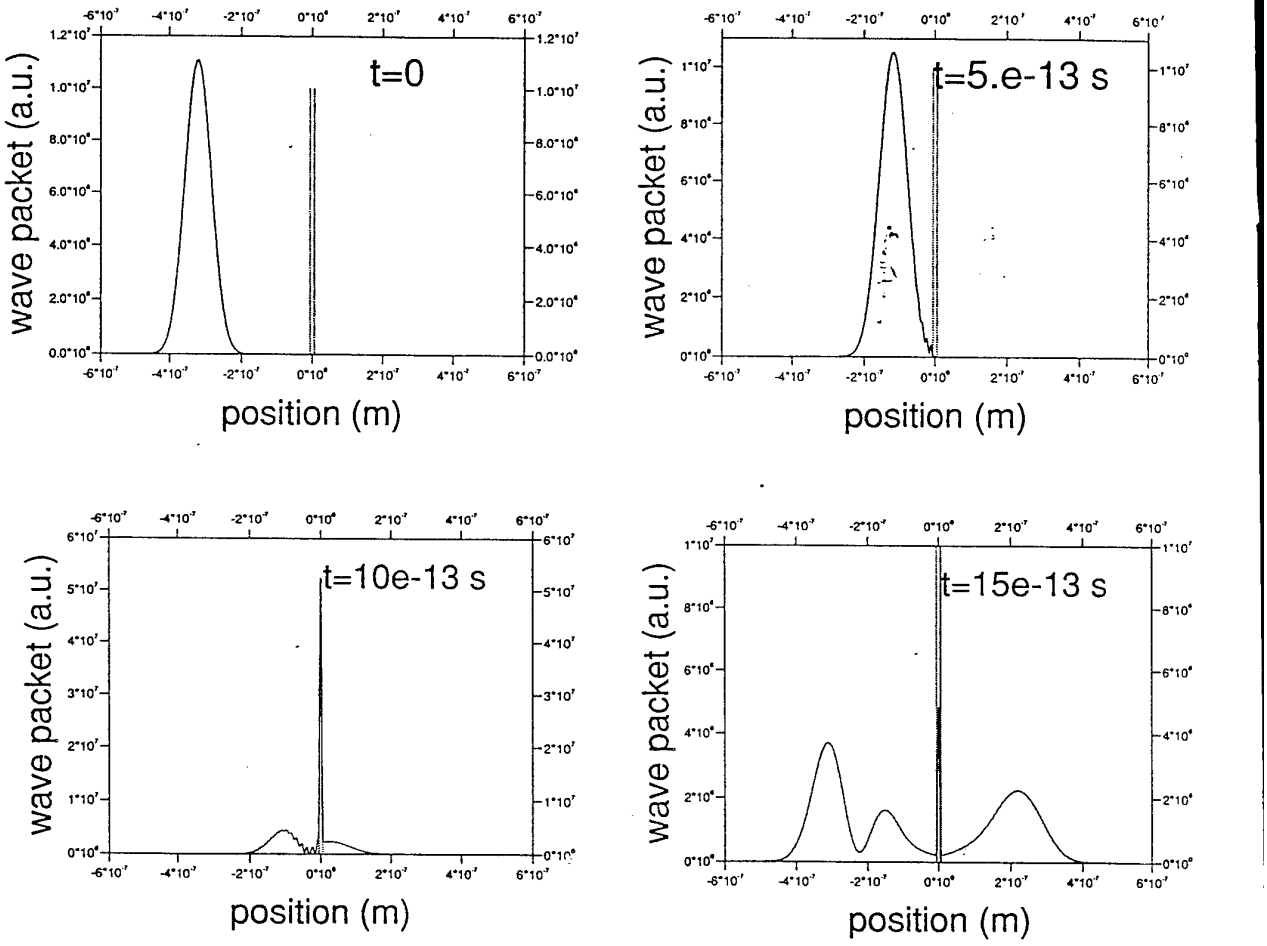

Fig. 4.1: Evolution of the electron wave packet propagating across a double barrier. The energy of the wave packet is centered around a resonance value of the doubl barrier.

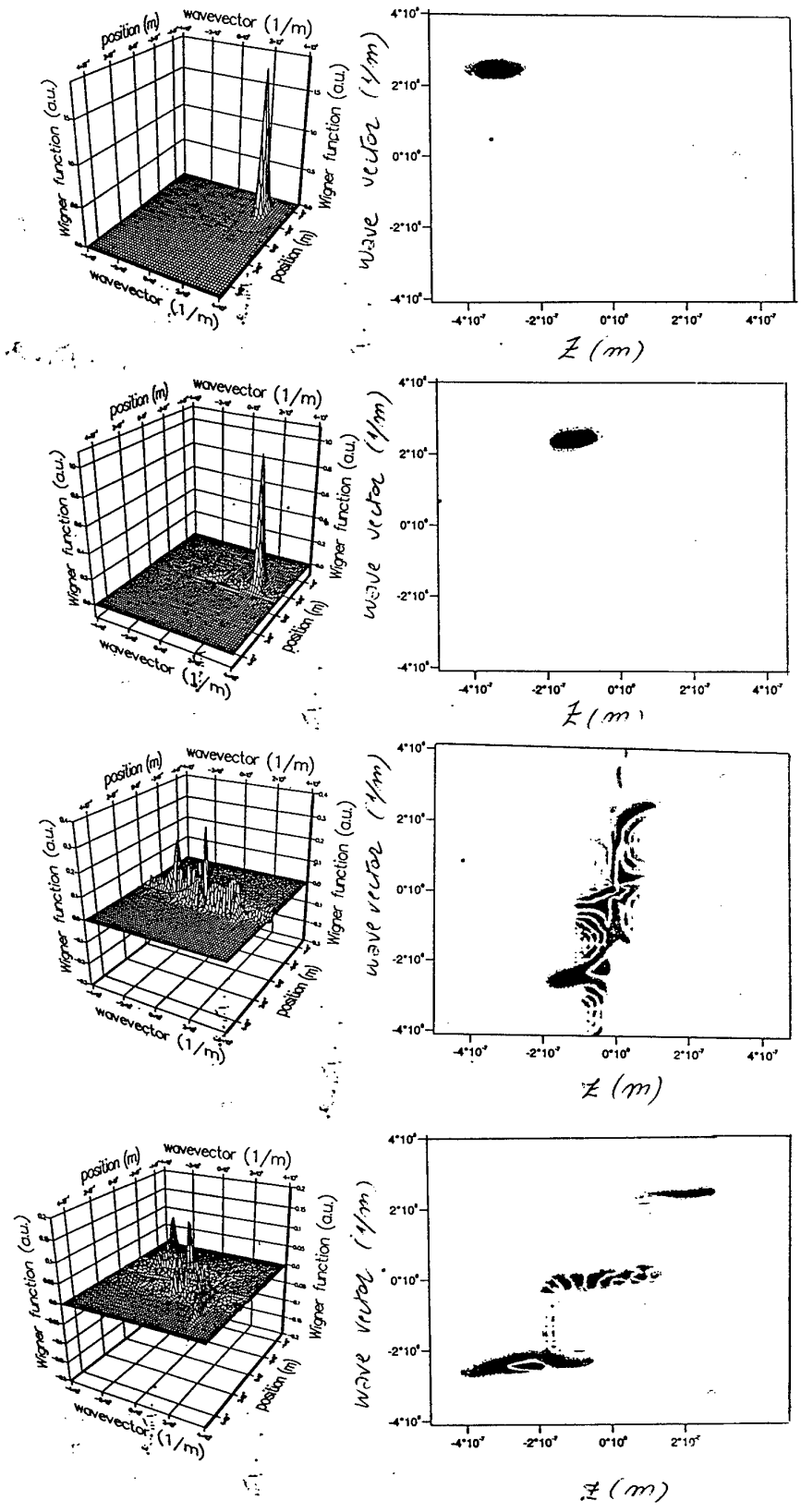

Fig. 4.2: Evolution of the wigner function for the wave packet shown in Fig. 4.2.

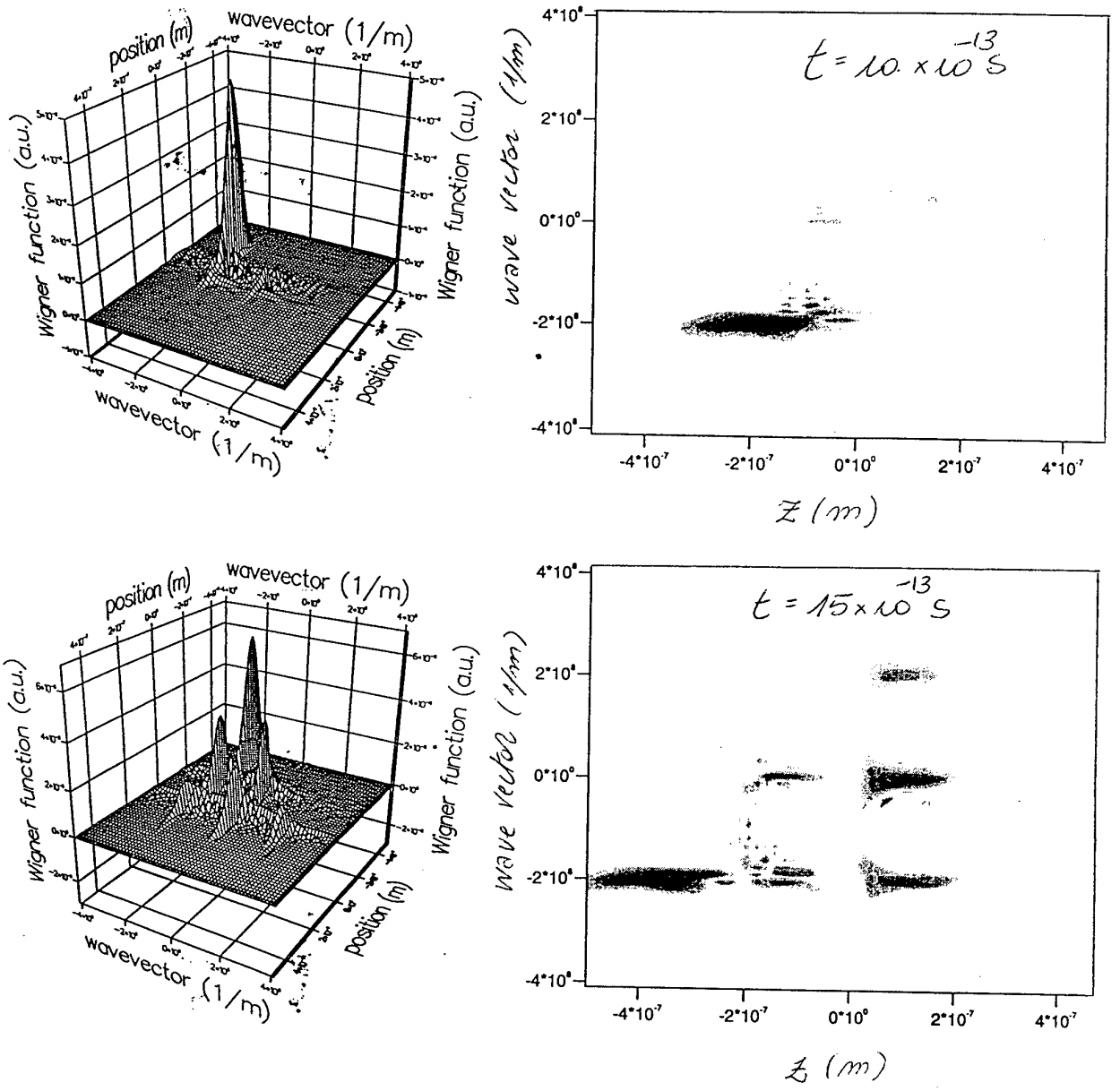

Fig. 4.3: Wigner function of the scattered wave packet during the scattering process.

5. Coherent transport in two-dimensional systems

Also for the two-dimensional case, the final goal is the determination of the Wigner function evolution, as described for the one-dimensional case. However, the numerical problems, already severe for that case, are in this case amplified. For this reason, for the time being only 2D coherent analysis have been performed, waiting to borrow the theoretical results and the numerical techniques from the 1D case once they will be assessed.

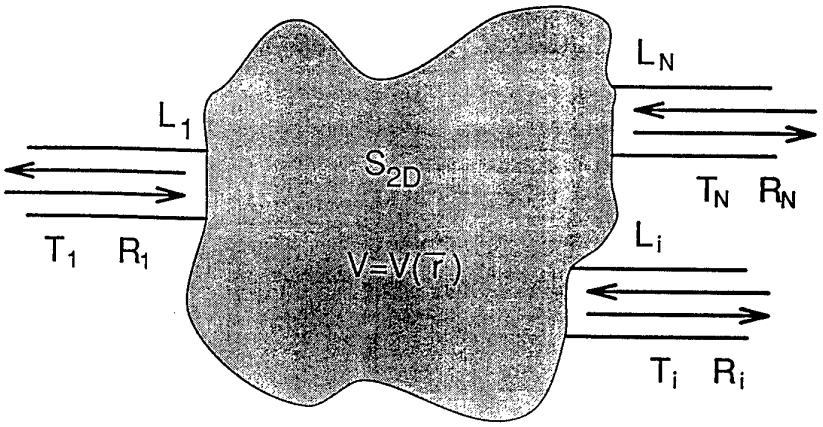

Fig. 5.1: Schematic representation of a 2D open-boundary system.

In the 2D case the time independent envelope-function equation has been solved in a generic 2D open boundary system. Fig. 5.1 shows a generic 2D open-boundary system. It consists of a 2D internal region where a 2D potential profile is present. The system boundary are all closed except those with the system leads, i.e. the channel of infinite length and finite width through which the system exchanges charge with the external world.

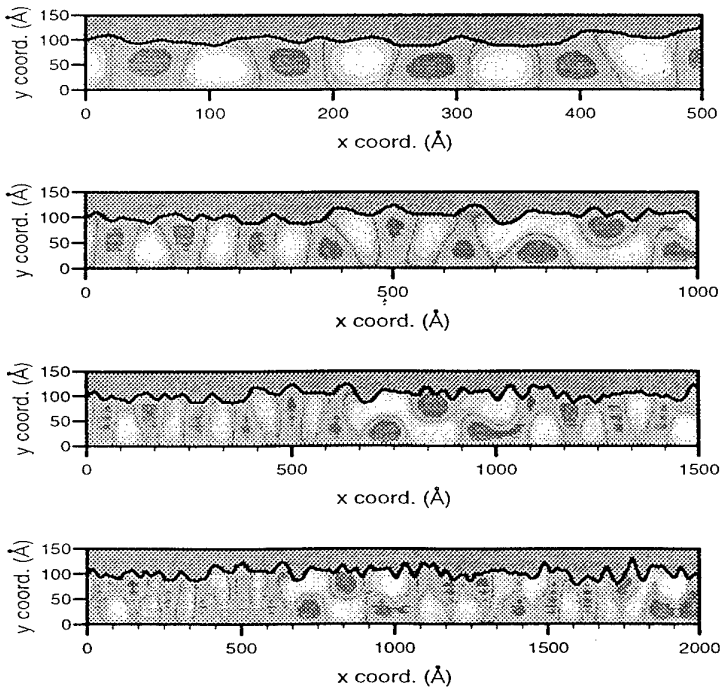

Fig. 5.2: Wave function propagation through rough channels of different length.

The solution is computed imposing zero wave function at the border of the region and a superposition of incoming and reflected plane waves and evanescent modes at each lead boundary.The finite elements scheme over a triangular mesh has been used.

The simulator has been applied to the study of the transmission properties of a resonant cavity with a localized screened Coulomb potential, simulating the presence of a dopant impurity, and of rough channels of different lengths.

As an example, in Fig. 5.2 and Fig. 5.3 the propagation through rough channels of different length is reported. Fig. 5.2 shows the localization effect occurring in a quantum channel (i.e. a MOSFET one) due to

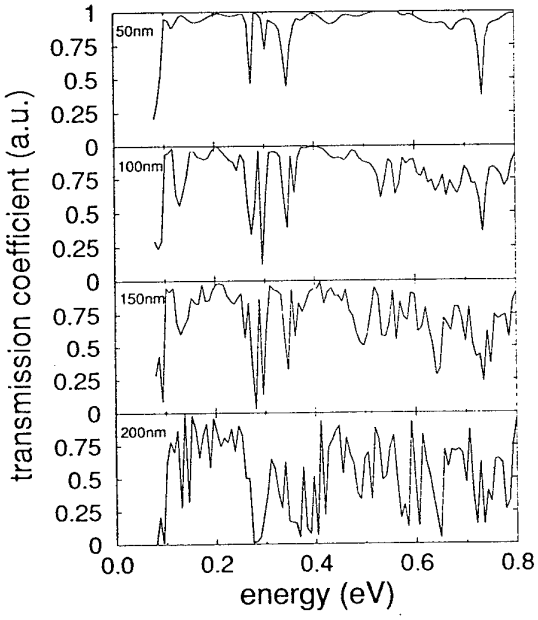

Fig. 5.3: Transmission coefficients vs. energy for the quantum channels of Fig. 5.2.

the surface roughness. This directly reflects in the transmissivity of the channel, as can be seen in Fig. 5.3.

Furthermore, the analysis of the transit time of a coherent wave has been carried out. The goal is to find a figure of merit to compare the performance of different structures when coherent transport takes places. A generalization to the two-dimensional case of the "phase time" has been developed:

$$\Delta\tau = \frac{m}{\hbar}\left(\frac{\sum_i T_i}{\sum_i T_i\, k_i}\, b - \frac{a}{k_I} + \frac{1}{k_I}\,\frac{\sum_i T_i\, k_i\, \beta'_i}{\sum_i T_i\, k_i}\right)$$

where I and i indicate the mode entering and exiting the system, respectively; T_i is the transmission coefficient; k are the wave vectors; β_i' the derivative of the phase of the outgoing wave with respect to k_i; a and b are the system limits.

We have applied the derived definition of phase time to simple cases of study, namely the determination of the propagation delay of electrons transiting through a quantum wire and a double-barrier resonant-tunneling diode, in presence of a single Coulomb scatterer.

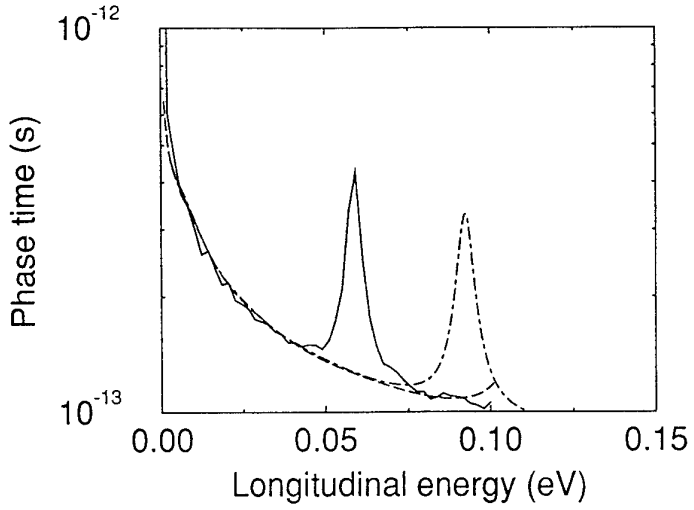

Fig. 5.4: Phase time through a double barrier resonant diode.

As an example, Fig. 5.4 shows the phase time behavior through a double barrier resonant diode.

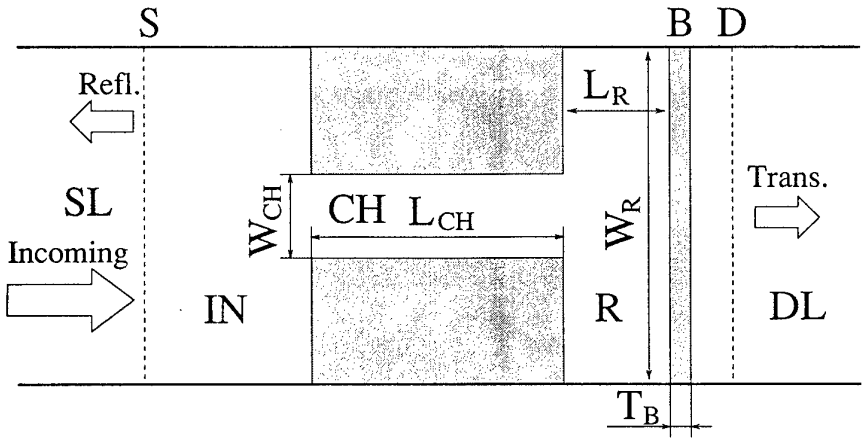

Fig. 5.5: Geometry of the investigated 2D tunneling device.

Still concerning the 2D coherent transport, the transmissivity of 2D tunneling structures has also been investigated. As a result, a new resonant condition has been discovered. In principle, the phenomenon is

similar to what observed in double-barrier resonant diodes, but in this case the resonance condition is determined by the 2D geometrical features of the system.

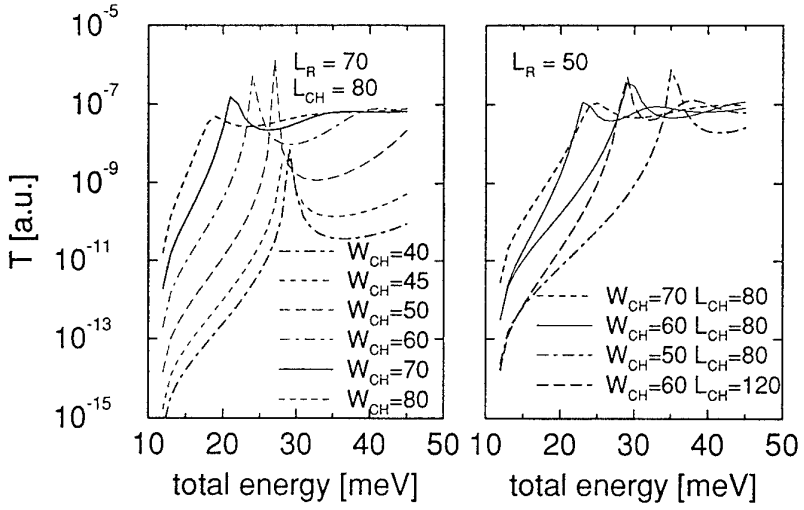

Fig. 5.6: Resonance transmissivity peaks for different geometrical configurations of the system of Fig. 5.6.

Fig. 5.5 shows the 2D gemetry of a resonating tunneling cavity, while Fig. 5.6 its transmissivity behavior for different values of the geometrical parameters of Fig. 5.5. We have found that the resonant energy

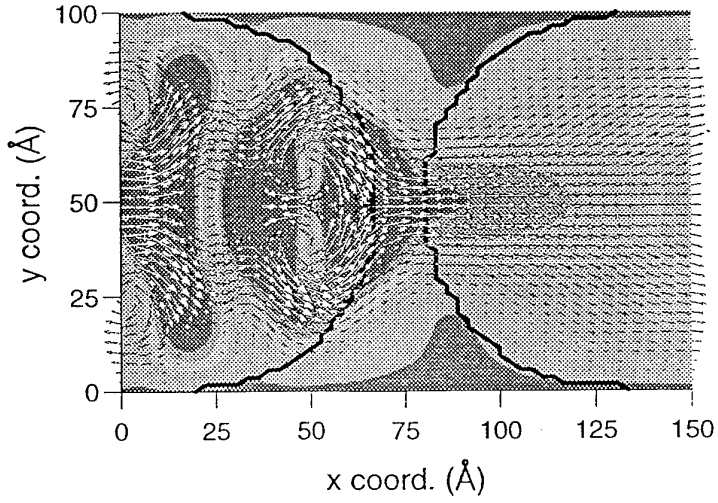

Fig. 5.7: Simulation of an electrostatic lens. Note the focusing effect taking place on the transmitted wave function. Arrows indicate the current density vectors.

corresponds to the energy of the corresponding closed boundary system at which the eigenstate peaks inside the resonating cavity just before the transverse potential barrier.

Another interesting 2D effect we have simulated is that of electron focusing through the use of a bo-concave-shaped potential barrier. Fig. 5.7 shows one of the simulation results.

6. Conclusions

In this final report we have illustrated the main results achieved under this contract.

On the theoretical side, the Wigner function formalism for quantum dynamics in mesoscopic systems has been developed.

From the application standpoint, one-dymensional systems dynamics has been analyzed including the effect of a single phonon scattering event. This as been done both for a wave packet and for scattering states.

As for the case of two-dimensional open-boundary systems, only coherent dynamics has been investigated so far. Interesting mesoscopic systems, such as rough quantized channels, elecroscatic lenses, and resonant tunneling cavities have been studied.

7. Publications

C. Jacoboni, R. Brunetti, M. Nedjalkov, ''Quantum transport with electron-phonon interaction in the Wigner-function formalism'', in HCIS IX Proceedings, in press.

A. Abramo, P. Casarini, C.Jacoboni, ''Transmission properties of resonant cavities and rough quantum wells'', in HCIS IX Proceedings, in press.

A. Abramo, P. Casarini, C. Jacoboni, , ''Phase time for coherent transport in two-dimensional structures'' , to be published on Appl. Phy. Lett., **69** (5), 1996.

C. Fiegna, A.Abramo ''Optimization of channel profiles for ultra-short MOSFETs by quantum simulation'', submitted to IEDM 1996.