Understandable algorithm for exchange interaction: quantum noise in nanoelectronic devices

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INTRODUCTION

Exchange interaction (only wave functions whose probability remains unchanged under permutations of electrons are acceptable) has a relevant role in many quantum phenomena. However, in nanoelectronic simulators, such interaction is directly ignored or substituted by the Pauli exclusion principle (two electrons can not occupy the same quantum state simultaneously). The direct implementation of this last principle faces many difficulties. *Do we have to avoid the possibility of injecting an electron from the left reservoir because there is one (with the same energy) in the right reservoir? Why?* Initially, electrons are separated and they do not suffer any exchange interaction. Only later, when their wave functions interact inside the active region, the exchange interaction appears (Fig.1). Avoiding the injection of electrons neglects the rich (Coulomb plus exchange) phenomenology that can appear inside the active region.

EXCHANGE INTERACTION FROM ANTISYMMETRY

In this conference, we present a novel algorithm that works directly with the antisymmetric wave function (the Pauli exclusion principle is just a particular consequence of the antisymmetry) and we test the validity and accuracy of our algorithm for quantum noise [1].

1) Electron injection model: We consider a typical (binomial) injection model for electrons [4]. It depends on the Fermi-Dirac function f_L at left contact and f_R at right. The idea of no correlation between left and right injection at the time of injection is preserved [4].

2) Time dependent evolution of electrons: In our model, electrons are described by different wave packets and their evolution is computed according to the time dependent Schrödinger equation with only an additional requirement, their (many-particle) wave function must be antisymmetric [4]. The time-evolution of the wave function itself determines, the probability of two different electrons being both reflected or both transmitted, and also the probabilities of one reflected and the other transmitted $\overline{TR}$ and $\overline{RT}$.

SIMPLE TEST: QUANTUM NOISE

For simple scenarios without Coulomb, quantum noise can be computed trivially from the variance of the number of electrons transmitted during τ [1]:

$$\langle S\rangle = lim_{\tau\to\infty} 2q^2 \frac{\langle N^2\rangle - \langle N\rangle^2}{\tau} \quad (1)$$

In particular, for two electrons injected from different sides with the same energy, looking at table 2, we get:

$$\langle N^2\rangle - \langle N\rangle^2 = T\{f_L(1-f_L) + f_R(1-f_R)\} + T(1-T)(f_L-f_R)^2 + (\overline{TR}+\overline{RT})f_L f_R \quad (2)$$

Finally, for a single-band injection (with a factor 2 for spin) with $(\tau)^{-1} = \Delta E/(\pi\hbar)$ and using (2) and (1):

$$\langle S\rangle = \frac{4q^2}{h}\int_0^\infty dE\,[T\{f_L(1-f_L) + f_R(1-f_R)\} + T(1-T)(f_L-f_R)^2 + 2\overline{TR}f_L f_R] \quad (3)$$

which exactly reproduces Büttiker noise [2] as seen in Fig. 3. In this figure it is also represented the expected noise for two distinguishable particles, which contains the "spurious" term $\overline{RT} = RT$. For scenarios, with an interplay between exchange, tunneling and Coulomb a rich phenomenology appears [4], [1] as seen in Figs. 4 and 5.

CONCLUSION

In conclusion, we present an quantum transport algorithm where exchange interaction is introduced as any additional interaction inside the active region. The approach is tested by computing quantum noise in simple system without Coulomb (where analytical results are known). The present approach can be applied also to more complicated scenarios, with and interplay of exchange, tunneling and Coulomb interactions [3], [4].

ISBN 978-2-9547858-0-6

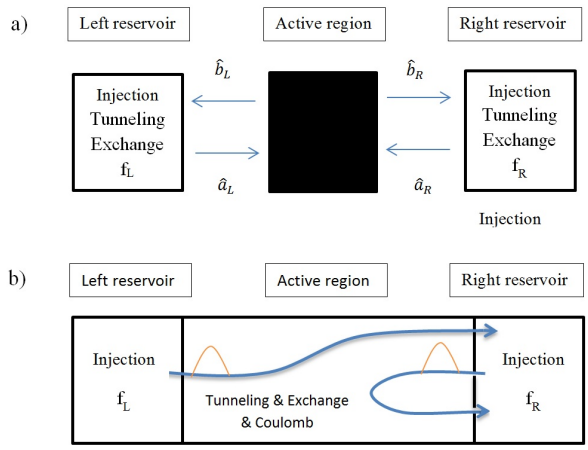

Fig. 1: (a) The second quantization approaches used for quantum noise computations [6]. The exchange interaction is introduced (though the Pauli principle) at the left and right reservoir, not in the active region. (b) A time-dependent approach [3], [4]. The exchange interaction is considered (through the wave function antisymmetry) inside the active region, not at the reservoirs.

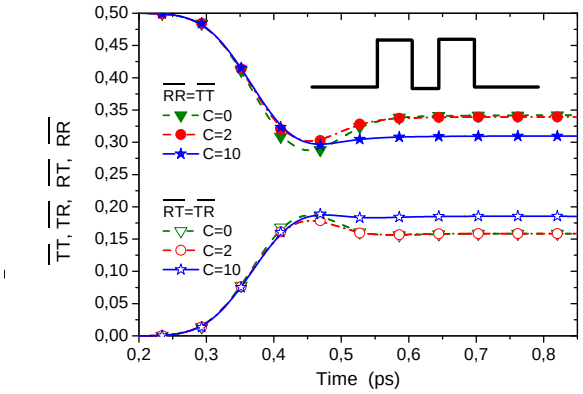

Fig. 4: Time evolution of $\overline{RR}, \overline{TT}$ (upper lines) and $\overline{RT}, \overline{TR}$ (lower lines) in Silicon double barrier (with exchange and Coulomb interaction). The wave packets dispersion is $50\ nm$. The inset shows the double barrier profile of 0.4 eV high, 0.8 nm long and the well length is 3.2nm. The system present a very rich phenomenology inaccessible from the analytical Büttiker expressions.

L / R		Injection: Transmitted	Injection: Reflected	No injection
Injection	Transmitted	$\overline{TT} f_L f_R$	$\overline{RT} f_L f_R$	$T(1-f_L)f_R$
		0	-1	-1
	Reflected	$\overline{TR} f_L f_R$	$\overline{RR} f_L f_R$	$R(1-f_L)f_R$
		1	0	0
No injection		$T f_L (1-f_R)$	$R f_L (1-f_R)$	$(1-f_L)(1-f_R)$
		1	0	0

Fig. 2: Probability $P(N,\tau)$ (upper) that N (lower) electrons with energy E have effectively been transmitted from left to right reservoir during the time interval τ. Such probabilities are computed from wave-packets by directly solving the time dependent Schrödinger equation with antisymmetry [1]

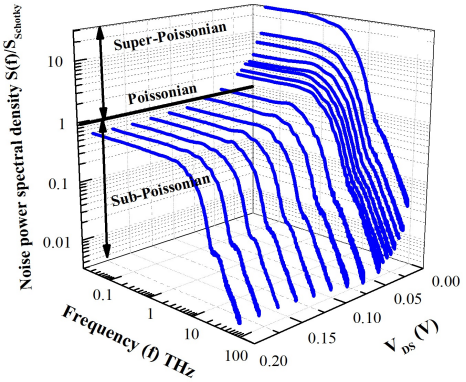

Fig. 5: A two-terminal simulation of a GaAs doped nano-resistor with exchange and Coulomb interaction of many (more than 2) particles using the BITLLES simulator [4]. The power spectral density of the noise (at zero and high frequency) are plotted for different applied voltage.

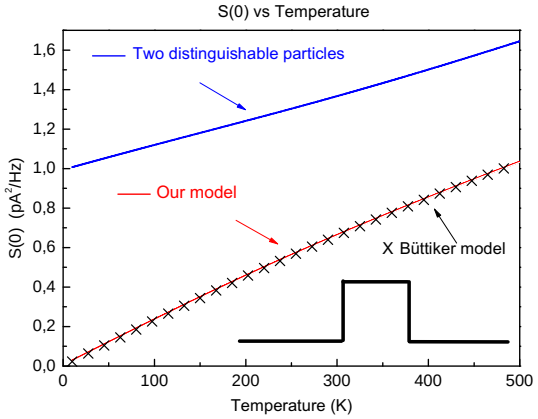

Fig. 3: Power spectral density of the thermal noise, at equilibrium, for electrons impinging in a single barrier potential of GaAs (with exchange but without Coulomb interaction). The agreement with Büttiker results are perfect. The wave packet dispersion is 50nm. The inset shows the potential profile, the barrier is 0.4 eV high and 0.8 nm long.

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