Tunneling time in nanostructures

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We review existing approaches to the problem of tunneling time, focussing on the Larmor clock approach. We develop a Green's function formalism and with it we are able to obtain close expressions for the tunneling and for the reflection times. A strong analogy between the results of the different approaches is established, and we show that their main differences are due to finite size effects. Furthermore we study the dwell time, and check that it can be exactly written as an average of one of the components of the traversal and the reflection times.We apply the results to a rectangular barrier, a periodic system and resonant tunneling, and we analyze the dependence of the tunneling time with the size of the wavepacket.

We also discuss the recharging time in chemical nanostructures like ligand stabilized micro-clusters. We show that for nanoparticles with very small tunneling resistance $R_T \leq 10^5\ \Omega$ it becomes to the same order of magnitude with tunneling time.

CONTENTS

I. INTRODUCTION

During the last few years key subjects and, consequently, terms in materials research have been continuously changing, indicating a tendency towards smaller and smaller scales. The physics of "low dimensional structures" was replaced by the discipline of "submicron physics", emphasizing the effects due to a reduction of size. Then the term "mesoscopic systems" was introduced referring to typical length–scales ranging from a few nanometers up to a few micrometers. More recently still, the terms "nanophase–" or "nanostructured materials" have become popular, indicating that scientists had learned to manipulate, synthesize, analyze and observe objects approaching the molecular and atomic scales.

Usually in the literature it was distinguished between "physical–" and "chemical nanostructures". Under the term "physical nanostructures" are classified all artificially built up structures, as obtained, for example, by evaporation and subsequent deposition of materials. On the other hand, the term "chemical nanostructures" comprises all those nanophase materials that can be obtained by methods of chemical synthesis, such as the chemical compounds with chain–like or layer type–structures, as well as the cluster compounds. A review of the electronic properties of nanophase materials obtained from chemical synthesis was recently given by de Jongh [1]. A survey of chemically synthesized metal clusters was edited by Schmid [2]. And the prospect of the applications of metal and semiconductor clusters in inorganic host structures was presented by Simon [3].

The question of the time spent by a particle in a given region of space is not new and has recently attracted a great deal of interest [4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16]. The problem has been approached from many different points of view, and there exists a huge literature on the tunneling problem of electrons through a barrier, although tunneling times have continued to be controversial even until now. As pointed out by Landauer and Martin [11], there is no clear consensus about simple expressions for the time in quantum mechanics (QM), where there is not an Hermitian operator associated with it. The problem of the tunneling time of single electrons (SE) in nanostructures or in mesoscopic systems smaller than 10 nm becomes even more complicated, due to the Coulomb blockade effects [17] on small amounts of electrons and discreteness of electric charge.

In the present paper we intended to review the theoretical approaches for tunneling times to illustrate the problems involved in nanostructures. But this plan proved to be more difficult than expected: although there exists an extended literature on tunneling times (see Landauer an Martin [11] and Hauge and Støvneng [4] and references therein), quantum-mechanical treatments mostly deal with propagating wavepackets in a more or less general way and they do not concentrate on tunneling times in nanostructures. As far as we know, there is not yet a proper treatment about tunneling times in very small nanostructures with single, localized electrons, where the radius of "localization" is in the same order of magnitude as the length of the barrier L. On the other hand, materials research and rapid systems development with nanostructures, particularly for microelectronic (ME) purposes (see Simon and Schön [18]), are claiming for an understanding of time constants or operation times [19] and the tunneling times involved.

Thus it proved to be necessary not simply to present the existing models and theories on tunneling time but to review them with respect to these necessities together with possible alternatives and to estimate future developments. In this context some original works will be analyzed from this point of view. We will be particularly concern with the closed analytical treatment based on Green's function formalism. With respect to ME, the very short recharging times for the most promising class of chemically size tailored nanoclusters will be included into the time discussion including possible consequences with superluminal velocities.

In this Introduction we will first recall some results about tunneling including consequences of "superluminal " speed. After reporting on SE–tunneling in nanostructures we are explaining usual terms related to tunneling times and the problem of defining velocities. Then we deal with the wavepacket approach and its limits. An introductory section about phase time and superluminal velocity in periodic nanostructures will be followed by remarks to time in Heisenberg's uncertainty relation.

In the main part of the paper we study the Larmor clock approach to tunneling time, based on measuring the spin rotation of an electron under a weak magnetic field acting on the region of interest. In section 3, we develop a Green's function formalism for the traversal and reflection times, based on the previous approach. We review the rest of the existing major approaches to the time problem in section 4. In section 5, the dwell time, which corresponds to the amount of time that a particle spend in a region independently of whether later is transmitted or reflected, is analyzed. Section 6 is devoted to the study of recharging time in nanostructures. In section 7, we present numerical results about the traversal time in rectangular barriers, periodic systems and resonant tunneling. We finally extract some conclusions and present open questions. We end with three technical appendices about Green's functions in layered systems, the corresponding transmission coefficients and the integrals of the Green's functions.

A Historical background on tunneling time

As mentioned above, tunneling refers to the classically impossible process of a particle or wave to penetrate an energy barrier when its energy is smaller than the maximum of the potential of the barrier. The main magnitudes involved in the problem are the height V_0 and the length L of the potential barrier. If they are large the probability to penetrate the barrier is very small and we say that it is an opaque barrier (for ME purposes). Examples of tunneling processes are α–decay, transmission of electromagnetic waves in undersized waveguides and tunneling of electrons. A quantum particle usually is said to have an intrinsic "wave nature", often paraphrased by "wave functions" or "wavepackets". The probability to penetrate a barrier, which is quantified through the transmission coefficient (probability) T, strongly depends on the nature of the exponential decay of the wave function under the barrier.

For many tunnel effects, the tunneling time is not of great practical interest, as for example in the case of radioactive decay. Likewise –until recently the tunneling of electromagnetic waves was not of great importance for ME. On the other hand, tunneling of electrons has been of utmost importance for all fast effects in ME. The first device used as a fast switch was the semiconductor tunnel-diode which was commercially introduced in the late fifties [20]. But again, only its total relaxation time was of interest and not the pure tunneling time through the bounding barrier.

Until relatively recently, little attention was paid to Hartman's theoretical work on tunneling time of wavepackets in the sixties [21]. His main striking result was that under certain circumstances (opaque barrier) the tunneling time is independent of L and the traversal time can be less than the time that would be required to travel a distance equal to L in vacuum. Similar results were found by Rybachenko [22] for electrons in a rectangular barrier. Although these were excellent pioneer works, 30 years ago time was not ripe for a further evaluation with respect to practical consequences in ME or even to philosophical ones. Additionally, many physicists hesitated to deal with Hartman's results since a very fast tunneling, or a zero tunneling time holds a serious consequence: the tunneling velocity or the average velocity may become higher than the light velocity c. Thus superluminal speed can be expected [23, 24] or measured in some cases like in experiments where electromagnetic waves pass through a barrier [25, 26, 27, 28, 29] or through an optical gap [9, 10, 16]. But superluminal speed goes beyond the limits of causality given by Einstein's relativity theory with its principle of constant of light velocity which in vacuum defines the simultaneity of time[118].

So far, the knowledge of different clocks in Macrocosm had no really important practical consequences on every day life. However superluminal tunneling speed affects causality in Microcosmos and the consequences are still unknown. In Microcosmos the possibility of quanta propagating with superluminal speed may have the following consequences:

- causality may be broken and, in theory, this makes more difficult Einstein's vision of a "unifying field theory", which even was deterministic.
- there are many philosophical and theoretical implications. In practice, we must analyze whether a signal transmitted by a superluminal microscopic channel, e.g., a nanostructure, still makes macroscopic sense.
- for nanoelectronics this problem will become a real one when dealing with single particles like electrons with, say, one de Broglie wavelength.

B Tunneling in nanostructures

Since SE tunneling processes could be evaluated in many nanostructures [31, 32, 33, 34], it provided a strong motive for advancing nanofabrication technologies and research on tunneling, which become important even at room temperature, since the operating temperature of single electron devices is directly related to the geometrical size of the electron localization. In SE the discreteness of the electric charge becomes essential and a quantum mechanical tunneling of electrons in a system of rather opaque junctions can be much affected by Coulomb interactions. For ME purposes the electron interactions, the barrier height and shape and thus the tunneling probability can be varied at will by externally applied voltages or by injected charges.

Many attempts have been made to advance lithography technology in the sub-10 nm range. But at present, the progress guided by the miniaturization of conventional electronic circuits has come to a standstill at the 100 nm range and fails to fully satisfy the requirements of SE [35]. Instead, quantum dots fabricated by physical or chemical methods are favored at present, mainly in hybrid-elements where sub-10 nm objects, chains or layers can be captured in gaps or grooves on the surface of conducting and non-conducting wafers, formed by the combination of electron beam lithography with the shadow evaporation or by spin coating [36, 37].

The possible electronic applications of chemically synthesized metal and/or semiconductor clusters in the sub-10 nm range surrounded by a protecting shell of organic ligands has been first discussed by Schön and Simon [33]. These ligand stabilized microclusters (e.g.Au_{55} with a diameter $D \approx 2$ nm, see fig.6b) can operate as quantum dots in so called building blocks for devices up to room temperatures. After their introduction, research on chemically size tailored nanostructures took a fast worldwide evolution (see Simon and Schön [18]) recently lead-

ing to the development of a single electron transistor using a molecularly linked gold colloidal particle chain [38]. In this technology the organic ligand molecules together with suitable spacer molecules [39] act as a chemically size tailored electron tunneling barrier and the cluster core as an electron localization site. Besides, there are attracting ideas how to exploit principles of SE for making logic and memory cells which in perspective could lead to assembling the computer "working "on single electrons [40].

With the above nanostructures, tailored chemically to our liking, ultrashort recharging times down to 10^{-15} *sec* are within reach (see 6.2.1). With all of these structures the problem of ultrashort tunneling times cannot be avoided any longer since operation times involve subbarrier tunneling and the wave nature of the electrons becomes an important property.

C Tunneling times and velocities

Usually in QM we can only measure quantities for which we have introduced a Hermitian operator, e.g., energy E, momentum p, coordinate y and so on. For these quantities, expectation values can be calculated and checked experimentally. However, time appears in the standard quantum mechanical approach only as a parameter and therefore its expectation value is not defined. Since the beginning of QM, people has been aware of the conceptual problem of how to introduce a time operator with an appropriate classical analog, and there have been different theoretical approaches to find a consistent description of this problem [4, 11, 41].

Moreover, according to QM a particle under a barrier, with energy E smaller then V_0, can only be observed with a strong inelastic influence. If we fix its coordinate with an accuracy of Δy smaller than the length of the barrier L, it necessarily results in a variation of momentum, caused by the measurement, and correspondingly in a change of the kinetic energy of the particle. This change in energy must be greater than the energy difference between the barrier height V_0 and the energy of the particle E [42]. If such a measurement would be carried out by a light quanta then we would have $\hbar\omega \geq V_0 - E$. The latter result demonstrates impressively that it is practically impossible to measure the propagation time from one coordinate (position) to the next under a barrier. This means that in practice one must try to observe the particle outside the barrier, say left or right of the region of interest. For short wavepackets, where the length of the wavepacket approaches the barrier length L this means "far" left and "far" right (see 7.2).

One can associate the traversal time with the time during which a transmitted particle interacts with the region of interest, as measured by some physical clock which can detect the particle's presence after leaving the region. For electrons, this approach can utilize the Larmor precession frequency of the spin produced by a weak magnetic field hypothetically acting within the barrier region [22, 43, 44, 45]. Similar procedures has been developed for electromagnetic waves in Ref. [46], where was proposed a clock based on the Faraday effect to measure their interaction time in a slab. Another approach is to calculate the traversal time of a particle through a barrier by following the behavior of a wavepacket and determine the delay due to the structure of the region. In this approach one has to be careful with the interpretation of the results, since, for example, an emerging peak is not necessarily related to the incident peak in a causative way [47]. For more discussions on this problem see e.g. Ref. [11] and references therein. Martin and Landauer [48] studied the problem of the traversal time of classical evanescent electromagnetic waves by following the behavior of a wavepacket in a waveguide, and Ruiz *et al.* [15, 49] analyzed their behavior in the optical gap of a periodic structure.

The above preliminary considerations show that it is difficult to write or talk with a well-defined meaning about the concept of tunneling time and that it is still an open question which definition of a delay time corresponds to the tunneling time of a photon or an electron. These difficulties have contributed to increase the number of terms related to "times" that have been introduced in the specialized literature, with more or less the same meaning. In what follows we review the terms we have encountered in the literature and we try to clarify their meaning and, sometimes subtle, differences. The first 8 terms are very similar and refer to the time it takes a wave to cross a barrier. In this article their use will slightly differ, depending on the theoretical and physical context.

1. Phase Time. It emphasizes that it is obtained from the phase of the transmission amplitude. It does not correspond to a time related to the phase velocity.

2. Delay Time. It focuses on the kinematic aspects of wavepacket propagation, rather than on interactions with the barrier.

3. Tunneling Time. It is the crossing time for energies below the barrier potential, i.e., for evanescent waves.

4. Traversal Time. General expression of the crossing time of a given region.

5. Transmission Time. The same as above.

6. Barrier Interaction Time. It emphasizes the fact that tunneling also means interaction with the barrier.

7. Sub–Barrier Tunneling Time. It reminds us the fact that we must always make comparisons with the time that a particle would need when propagating above the barrier or in free space.

8. Büttiker-Landauer Time. We will see that then the tunneling time has two components, one τ_y depending of the density of states and the other τ_z related to the resistance. The Büttiker-Landauer time refers to the square root of the sum of the squares of both components. It also denotes that, for the calculation of tunneling times, one needs physical and mathematical models, like the above explained clocks.

9. Dwell Time. It is widely accepted as the average time spent by a particle in a given region of space. It tells us how many electrons are 'dwelling' at the same time under a barrier. It is important for applications in ME since the number of electrons in SE is small.

10. Reflection Time. It plays the same role as the traversal time, but for electrons reflected at the barrier. It can be calculated analogously to the tunneling time by means of spin orientation with the Larmor clock method, etc. Reflection times may become an important quantity for applications in nanoelectronics, since there we find an architecture of arrangements of quantum wells for electron localization by pairs, chains or layers of quantum dots with tunneling barriers in between. If then, working electrons will be reflected from the barriers and back into the quantum well, the reflection time becomes important for recharging.

11. Recharging Time. This and the next two times must be discussed together, because in nanostructures all these three times –although being qualitatively different– may be of the same order of magnitude, approximately 10^{-15} *sec*, and in practice it is difficult to distinguish between them.

12. Ultrashort or Fast Tunneling Time.

13. Uncertainty Time. Looking for example at the smallest possible switch built up of a pair of two quantum dots by gold-clusters (see 6.2.3, fig.11) with relatively low tunneling resistance in between, the above, extremely fast "Recharging Time" can be determined. On the other hand, since within this time interval one electron tunnels between the two quantum dots, the concept of "Ultrashort Tunneling Time" must be involved. Since "Uncertainty Time" denotes electron fluctuations within the cluster core or between the two clusters when the tunneling resistance amounts to the resistance quantum, it must be included into the discussion. The problem is that at present nobody can separate these three times (e.g., as a sum) and it is an open question which time scale is relevant for ultrashort tunneling in nanostructures. Moreover, the smaller the structure and the barrier region, the more influence present the boundary conditions. We will show that for low energies the time components are mainly governed by boundary region terms (see also fig.4)). But again one cannot separate or calculate for a given nanostructure the boundary region times.

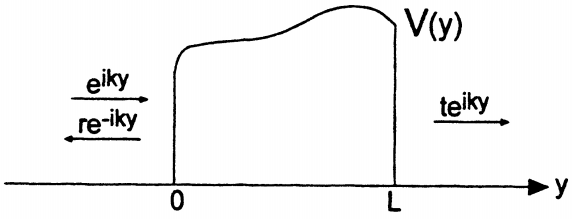

FIG. 1: One–dimensional stationary problem with a general barrier $V(y)$. A plain wave incident from the left is partly transmitted and partly reflected.

The problem of defining velocities is equally complicated as that of determining the time. One cannot use just one definition for the velocity both inside and outside the barrier at the same time. Usually, for a quantum particle when going from sub-barrier region to above-barrier region one can do analytical continuation of the wave function. But in the first case there is an exponential decay of the wave function and in the second case we deal with a free propagation of the electron and so a wave function with oscillations. This analytical continuation is not correct for the velocity under the barrier, because one gets an imaginary velocity. So there is no definition of velocity for sub–barrier regions and as a consequence, in the limit of an opaque barrier or in the forbidden gap of a periodic systems, it may be observed a "superluminal " speed.

D Wavepacket approach and limits

The simplest model which illustrates the tunneling problem for a quantum particle is a plane wave incident on a one–dimensional (1D) barrier (see fig.1). Part of the plane wave is reflected and part is transmitted. The above plane wave, which represents the electron in our model, is by nature infinitively large in space. The discussion of whether wavepackets with an infinite extension model the wave function of single photons or electrons and of whether they might be interpreted as signals is complicated [4, 11] and important for ME with nanostructures. Therefore it is better to consider a finite wavepacket and to look at its peak evolution in time (see fig.2).

Thus the phase time is the time which elapses between the peak of the wavepacket entering the barrier and leaving it and can be defined as the energy derivative of the

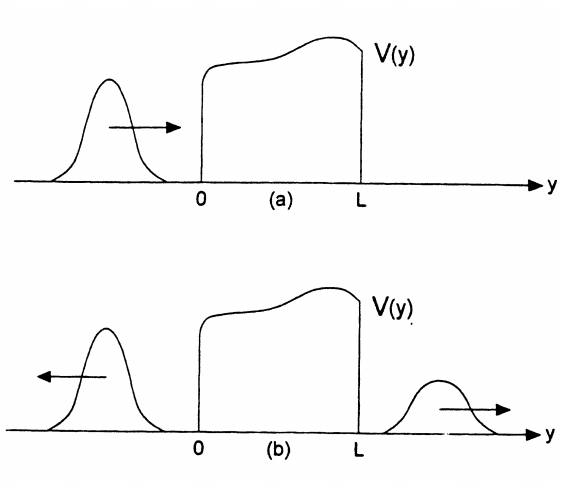

FIG. 2: a) The initial wavepacket incides from the left onto the barrier. b) Transmitted and reflected wavepackets are moving away from the barrier in opposite directions.

phase:

$$\tau_\varphi = \hbar \frac{d\varphi}{dE}. \tag{1}$$

In some cases this time can be easily calculated but as was mentioned before it will lead us to Hartman's effect. We will see (section 2) that, in general, more than one tunneling time are involved in the problem: τ_y, τ_z and the so–called Büttiker–Landauer $\tau^{\mathrm{BL}} = \sqrt{(\tau_y)^2 + (\tau_z)^2}$. Unfortunately this time is not additive in the sense, that when dividing the length of the barrier $L(y)$ arbitrarily into different parts, the total τ^{BL} tunneling time is not the sum of the individual tunneling times.

To illustrate consequences from the above wavepacket model let us consider a sharply peaked Gaussian wavepacket in space which starts to incide very far from the barrier to exclude any interaction. A wavepacket is an overlap of many plane waves with different wave numbers k. Hence, one may imagine the wavepacket as something like a group of electrons with different energies and velocities. The propagation will be dispersive and as a consequence the high-energy components of the packet will reach the barrier first. Due to the fact that higher energies can be transmitted more effectively than the low-energy components, the peak of the transmitted packet can leave the barrier long before the peak of the incident packet has arrived [50].

But what is really surprising is that even for the sub-barrier tunneling, i.e., when the wavepacket contains no energy components with energies above the rectangular barrier of height V_0, the transmitted packet will have a higher mean velocity than the free space propagation velocity. Numerical simulations show that one obtains very short tunneling times when the spread of the Gaussian wavepacket is larger than the barrier width L. Within these restrictions even the simple rectangular barrier is an "electron accelerator". This is a manifestation of the before mentioned Hartman effect (see section 2) which was treated by Rybachenko [22] for spin particles with analogous results. As we will show (section 2), the tunneling time component τ_y is independent of L and can be less than the time that would be required for a free particle to travel a distance equal to the barrier thickness L.

As a matter of principle, in ME for high information data rate, the spread of the Gaussian wavepacket must be small. Tunneling time(s) then will depend to a higher degree on the size of the incident wavepacket and the shape of the barrier: tunneling will become more sensitive to boundary effects at the barrier. For this reason we include a section about short wavepackets (see 7.2).

For the future SE logics in nanostructures, "pure " quantum mechanical properties of monochromatic single electrons with an energy less than 1 eV will be predominant. For such particles the de Broglie wavelength $\lambda_B = \hbar/p$ will be in the same order of magnitude as the length of the barrier. At the same time, this wavelength will be comparable to the radius of localization (e.g. for electrons confined in the core of ligand stabilized microclusters) in switches or mass memories (stores). Physically speaking this means that the picture of a dispersive wavepacket is now failing. As far as we know, fast tunneling for this case has not been treated theoretically until now.

E Phase time and superluminal velocity in periodic nanostructures

In ME the simultaneous transmission of electrons and of microwavepackets of selected optical signals between integrated microchips on wafers are of great importance and today much attention is paid to optoelectronics. Since on the way to future ultimate miniaturization, the present generation of devices hopefully will be replaced by nanostructured systems.

While at the end of the preceding section we sketched the problems with localized electrons for the future SE logics in nanostructures, in the present section we first pay attention to microwaves in undersized waveguide barrier-systems and then to photons propagating in 1D periodic and quasiperiodic Fibonacci and Thue–Morse systems. We briefly report about the former first "superluminal " experiment, but we are mainly interested into the latter as there exists a considerable analogy between these periodic systems and e.g. chains of the above chemical nanostructures. So there also must exist forbidden band gaps where electrons may propagate with "superluminal " speed. It must be noted that periodic structures can be easily built up in crystals of ligand-stabilized microclusters or likewise in chains or layers of supported cluster arrangements on structured wafers or

other substrates or even in channels or layer spaces of porous chemical nanostructures (see Simon and Schön [18]; see also fig.10). Some of these cluster arrangements are discussed in section 6.

In order to avoid the problems involved with the dispersive nature of the electron's wavepacket and the invasive measuring process in QM, it was easier to look at a gaussian wavepacket of classical electromagnetic waves and to try to measure the delay time at a barrier. Indeed, in most of the past tunneling experiments, instead of electrons, electromagnetic waves were used [8, 25], to exclude any electronic interaction with the tunneling barrier. The analogy between the time independent forms of the Schrödinger and the Maxwell equations confronts us again with Hartman's case: the possibility of achieving extremely high tunneling velocities, even superluminal velocities.

Thus looking back, it was not so surprising that the actual discussion on "superluminal " speed started almost at the same time with the series of microwaves experiments by transmission through systems consisting of undersized waveguides [7, 8, 25, 26, 27, 28, 29]. Steinberg *et al.* [9] found "superluminal" velocities for electromagnetic waves in the photonic band gap of multilayer dielectric mirrors. Spielman *et al.* [10] observed that the barrier traversal time of electromagnetic wavepacket tends to become independent of the barrier thickness for opaque barriers. This phenomena is closely related to Hartman's theoretical prediction for electron tunneling [21]. The theoretical explanation of this phenomena can be found in the framework of classical Maxwell equations by following the time evolution of the wavepacket in time, as it was mentioned above (see e.g. Refs.[24, 45, 49]). It was clear that parts of the microwavepacket were able to propagate with "superluminal " speed, proving the practical use of Hartman's effect.

The propagation of electromagnetic waves in 1D quasiperiodic Fibonacci and Thue–Morse systems was studied in [14]. It was shown, that, under certain conditions, again the phase time becomes independent of the system size and so "superluminal " group velocities can be obtained for very–narrow frequency band wavepackets.

With respect to the introductory remarks about the similarity between chains of multilayer dielectric systems and chemical nanostructures, the GF approach also will be used to study the tunneling time problem in functional systems approaching the molecular and atomic scales [51].

F Remarks to time in Heisenberg's uncertainty relation

An infinitely short tunneling time, corresponding to the Hartman's case or to a gap in a periodic structure, would imply a huge energy uncertainty according to the Heisenberg uncertainty relation applied to time and energy:

$$\Delta E \Delta t \geq \frac{\hbar}{2}. \tag{2}$$

There is a clear contradiction if in the tunneling process one associates the energy uncertainty with the change in energy. For elastic tunneling ($T + R = 1$), where the energy loss for each component of the electron's wavepacket is zero, one would then gets infinitively long times! So what is the answer for the old question of "How much time does tunneling take"? Is it anywhere between zero and infinity or does it depend on the quantity one measures in an experiment?

As mentioned at the beginning (see 1.3), usually in QM one can measure only quantities for which exists a Hermitian operator like energy, momentum and so on. For these, expectation values can be calculated and experimentally verified. However within conventional interpretations of QM concepts, time appears only as a parameter and thus an expectation value of time is not defined [41]. It is interesting to note that Heisenberg did not derive the previous uncertainty relation, but found it from complementarity in optics, where $\Delta\nu\Delta t \sim 1$ (see Born [52]). From $E = h\nu$, he deduced the above formulation, Eq. (2), of the uncertainty principle. Later Schrödinger derived it for any orthogonal functions, e.g., $\Delta p \Delta y \geq \hbar/2$. In general uncertainty relations can be derived for operators (belonging to physical quantities) which are not commutative. They follow from the existence of wave functions and average values defined by them. Furthermore they are independent of the special form of the Hamiltonian operator (see [53]). So, strictly speaking, nothing about tunneling time can be said from Heisenberg's uncertainty relation, since one only can consider relations like Eq.(2), but without time. Instead we can discuss relation with average kinetic energy and the square of locus. The latter results from a preliminary stage which one gets for the average kinetic energy $\bar{E}_{\rm kin}$ when deriving Heisenberg's relation:

$$\bar{E}_{\rm kin} \geq \frac{\hbar^2}{8m(\Delta y)^2} \tag{3}$$

One may use this equation to explain the stability of the hydrogen atom, which follows the differential equation of the harmonic oscillator.

Since in nanoelectronics single electrons mostly are starting out of quantum wells, e.g. when they are localized in microclusters, similar explanations as for the hydrogen atom may become important as well for the pure tunneling problem and for the tunneling of electrons from (out of) clusters. The only difference with respect to an atom is that now the electrons are not located in atomic orbitals but in cluster orbitals [33], and we have now the problem of harmonic oscillators without a central force.

We will shortly sketch the line of thought: the greater the average kinetic energy, the smaller the average square of variation Δy, which refers to the scope of motion of the electron. If D is the diameter of the nanoparticle (smaller than 2 nm for Au_{55}-clusters) then Δy is in the same order of magnitude and so $\bar{E}_{\rm kin} \approx D^{-2}$ and the average potential energy $\bar{E}_{\rm pot} \approx D^{-1}$. For small D the kinetic energy outweighs the potential energy, thus resulting in a "repulsion" from potential force: the confinement e.g. in a microcluster core will loosen, the electron knocks at the walls of the quantum well which may represent a tunnel barrier to a neighboring cluster (see fig.12 of the two cluster switch). In other words, the nearer an electron approaches the barrier, the higher the kinetic energy and thus the greater the chance to pass.

II. LARMOR CLOCK APPROACH

In 1967, Baz' [43, 44] proposed the use of the Larmor precession as a clock ticking off the time spent by a spin 1/2 particle inside a sphere of radius $r = a$. His idea was to consider the effect of a weak homogeneous magnetic field $\mathbf{B}$ on an incident beam of particles. Following the idea of Baz' let us suppose that inside the sphere $r = a$ there is a weak homogeneous magnetic field $\mathbf{B}$ directed along the z axis and which is zero for $r > a$. The incoming particles have a mass m and a kinetic energy $E = \hbar^2 k^2/2m$ and they move along the y axis with their spin polarized along the x axis (so that their magnetic moments μ are aligned along the x axis). As long as a particle stay outside the sphere, there are no forces acting on the magnetic moment and its direction remains unchanged. However, as soon as the particle enters the sphere, where a magnetic field is present, its magnetic moment will start precessing about the field vector with the well-known Larmor frequency

$$\omega_{\rm L} = 2\mu B/\hbar. \tag{4}$$

The precession will go on as long as the particle remains inside the sphere. The polarization of the transmitted (and reflected) particles is compared with the polarization of the incident particles. The angle $\theta_\perp$ in the plane xy, perpendicular to the magnetic field, between the initial and final polarizations is assumed to be given, in the lowest order in the field, by the Larmor frequency $\omega_{\rm L}$ multiplied by the time τ_y spent by the particle in the sphere

$$\theta_\perp = \varphi_{\rm L}\tau_y. \tag{5}$$

The change in polarization thus constitutes a Larmor clock to measure the interaction time of the particles with the region of interest.

Rybachenko [22], following the method of Baz', considered the simpler problem of the interaction time of particles with a one-dimensional (1D) rectangular barrier of height V_0 and width L, for which everything can be calculated analytically. For energies smaller than the height of the barrier, $E < V_0$, and for the important case of an opaque barrier, where there is a strong exponential decay of the wave function, Rybachenko found for the expectation value of the spin components of transmitted particles, to lowest order in the field $\mathbf{B}$, the following result:

$$\langle S_x\rangle \cong \frac{\hbar}{2}, \tag{6}$$

$$\langle S_y\rangle \cong -\frac{\hbar}{2}\,\omega_{\rm L}\tau_y \tag{7}$$

where τ_y is a characteristic interaction time given by

$$\tau_y = \frac{\hbar k}{V_0\xi}, \tag{8}$$

and ξ is the inverse decay length in the rectangular barrier

$$\xi = (k_0^2 - k^2)^{1/2} \tag{9}$$

with $k_0 = (2mV_0)^{1/2}/\hbar$. Here we have assumed that the direction of the field and of propagation of the particles are the same as defined at the beginning of the section. Rybachenko thought that the spin, in first order in the field, remains in the xy plane and so $\langle S_z\rangle = 0$.

Note that the characteristic time τ_y is independent of the barrier thickness L. Instead of being proportional to the length L is proportional to the decay length. For an opaque barrier this decay length can become very short and so τ_y can be very small, in fact, smaller than the time that would be required for the incident particle to travel a distance L in the absence of the barrier. A similar result was found by Hartman [21] analyzing the tunneling of a wavepacket through a rectangular potential barrier, which is known as Hartman's effect.

Hagmann [54] also arrived to the previous result, Eq. (8), by a curious argument related to the uncertainty principle. He assumed that the particle cross the barrier by borrowing certain energy ΔE during a time interval τ. Eq. (8) precisely corresponds to the time that minimizes the product $\tau\Delta E$.

In the method proposed by Baz' [43, 44], and in the one wort out by Rybachenko [22], the change in energy of the particle, due to the interaction $-\mu\mathbf{B}$, is assumed negligible for a small magnetic field $\mathbf{B}$ and there is no induced spin component parallel to the field. However, as we will see, the particles also acquire a spin component parallel to the field, even to first order in the field, due to the fact that particles with spin parallel to the field have a higher transmission probability than particles with spin antiparallel to the field.

A Büttiker analysis

Büttiker [45] presented a detailed analysis of the Larmor clock for the case of a 1D rectangular barrier. He

concluded that the main effect of the magnetic field is to tend to align the spin parallel to the magnetic field in order to minimize its energy (Zeeman effect). It means that a particle tunneling through a barrier in a magnetic field does not only perform a Larmor precession, but also a spin rotation produced by the Zeeman effect, which necessarily has to be included in the formalism.

The idea behind this Zeeman rotation is the following. A beam of particles polarized in the x direction can be represented as a mixture of particles with their z component equal to $\hbar/2$ with probability $1/2$ and equal to $-\hbar/2$ with probability $1/2$. Outside the barrier the particles have a kinetic energy E independent of the spin. But in the barrier the kinetic energy differs by the Zeeman contribution $\pm\hbar\omega_{\rm L}/2$, giving rise to a different exponential decay of the wave function depending on its spin component along the direction of the magnetic field. In the limit of small fields we have

$$\xi_{\pm} = \left(k_0^2 - k^2 \mp \frac{m\omega_{\rm L}}{\hbar}\right)^{1/2} \cong \xi \mp \frac{m\omega_{\rm L}}{2\hbar\xi} \tag{10}$$

where the sign indicates whether the z component of the spin is parallel $(+)$ or antiparallel $(-)$ to the field. Since $\xi_+ < \xi_-$, the particles with spin $\hbar/2$ will penetrate the barrier more easily than the particles with spin $-\hbar/2$, and so the transmitted particles will have a net z component of the spin. This net component of the spin along the direction of the field defines a second characteristic time τ_z of the particle in the barrier.

Büttiker assumed that the relevant interaction time depends on the times associated to both effects, the Larmor precession and the Zeeman splitting, and is given by

$$\tau^{\rm BL} = \left\{(\tau_y^{\rm BL})^2 + (\tau_z^{\rm BL})^2\right\}^{1/2} = \frac{\{\theta_\perp^2 + \theta_\parallel^2\}^{1/2}}{\omega_{\rm L}}. \tag{11}$$

Here $\theta_\parallel$ is the angle through which the expectation value of the spin in the transmitted beam is turned towards the magnetic field direction because of the difference in transmission probabilities for spin up ($S_z = +\hbar/2$) and spin down ($S_z = -\hbar/2$) particles. The traversal time defined by the previous equation is the so called Büttiker–Landauer (BL) time for transmitted particles. Although it was obtained in the context of tunneling, it is a general definition which applies for the traversal time of a particle or an electromagnetic wave through any given region of space.

The mathematical analysis of the problem is based on the standard expressions for the spin expectation values $\langle S_x\rangle$, $\langle S_y\rangle$ and $\langle S_z\rangle$ of a transmitted particle for arbitrary field strength B and potential barrier $V(y)$ confined to a finite segment $0 < y < L$ [45]:

$$\langle S_x\rangle = \frac{\hbar}{2}\left\langle \widehat{\Psi}\left|\sigma_x\right|\widehat{\Psi}\right\rangle = \frac{\hbar}{2}\frac{t_+t_-^* + t_+^*t_-}{|t_+|^2 + |t_-|^2} \tag{12}$$

$$\langle S_y\rangle = \frac{\hbar}{2}\left\langle \widehat{\Psi}\left|\sigma_y\right|\widehat{\Psi}\right\rangle = i\frac{\hbar}{2}\frac{t_+t_-^* - t_+^*t_-}{|t_+|^2 + |t_-|^2} \tag{13}$$

$$\langle S_z\rangle = \frac{\hbar}{2}\left\langle \widehat{\Psi}\left|\sigma_z\right|\widehat{\Psi}\right\rangle = \frac{\hbar}{2}\frac{|t_+|^2 - |t_-|^2}{|t_+|^2 + |t_-|^2} \tag{14}$$

where σ_x, σ_y, and σ_z are the Pauli spin matrices and the spinor $\widehat{\Psi}$ corresponds to (see the next section):

$$\widehat{\Psi} = \left(|t_+|^2 + |t_-|^2\right)^{-1/2}\begin{pmatrix} t_+ \\ t_- \end{pmatrix}. \tag{15}$$

where

$$t_{\pm} \equiv \sqrt{T_{\pm}}e^{i\varphi_{\pm}} \tag{16}$$

is the transmission amplitude for particles with $S_z = \pm\hbar/2$, and $T_\pm$ and $\varphi_\pm$ are the corresponding transmission coefficient and phase, respectively. For each of the spin components Büttiker defined a characteristic time describing the interaction of the tunneling particle with the barrier for an infinitesimal magnetic field:

$$\lim_{\omega_{\rm L}\to 0}\langle S_x\rangle = \frac{\hbar}{2}\left[1 - \frac{\omega_{\rm L}^2\left(\tau_x^{\rm BL}\right)^2}{2}\right], \tag{17}$$

$$\lim_{\omega_{\rm L}\to 0}\langle S_y\rangle = -\frac{\hbar}{2}\,\omega_{\rm L}\tau_y^{\rm BL}, \tag{18}$$

$$\lim_{\omega_{\rm L}\to 0}\langle S_z\rangle = \frac{\hbar}{2}\omega_{\rm L}\tau_z^{\rm BL}. \tag{19}$$

Only two of these characteristic times are independent. $\tau_x^{\rm BL}$, for example, can be obtained from $\tau_y^{\rm BL}$ and $\tau_z^{\rm BL}$ through the expression ${\tau_x^{\rm BL}}^2 = {\tau_y^{\rm BL}}^2 + {\tau_z^{\rm BL}}^2$, which can be deduced from the following relation between the spin components:

$$\langle S_x\rangle^2 + \langle S_y\rangle^2 + \langle S_z\rangle^2 = \frac{\hbar^2}{4}, \tag{20}$$

Below, we calculate $\tau_y^{\rm BL}$ and $\tau_z^{\rm BL}$ for a rectangular barrier, and in the next section we obtain their general expressions with the formalism of Green functions.

1 *Rectangular barrier*

For the special case of a 1D rectangular barrier, given by $V(y) = V_0\theta(y)\theta(L-y)$, it is possible to find exact analytical expressions for the time. For energies smaller than the height of the barrier, $E < V_0$, Büttiker [45] obtained the following expression for the characteristic time associated with the direction parallel to the field $\tau_z^{\rm BL}$:

$$\begin{aligned}\tau_z^{\rm BL} &= -\frac{m}{\hbar\xi}\frac{\partial \ln T^{1/2}}{\partial\xi} \\ &= \frac{mk_0^2}{\hbar\xi^2}\frac{\left(\xi^2 - k^2\right)\sinh^2(\xi L) + \left(\xi L k_0^2/2\right)\sinh(2\xi L)}{4k^2\xi^2 + k_0^2\sinh^2(\xi L)}.\end{aligned} \tag{21}$$

For the time $\tau_y^{\rm BL}$ associated with the direction of propagation, perpendicular to the field, he found:

$$\tau_y^{\rm BL} = -\frac{m}{\hbar\xi}\frac{\partial\varphi}{\partial\xi} = \frac{mk}{\hbar\xi}\frac{2\xi L\left(\xi^2-k^2\right)+k_0^2\sinh\left(2\xi L\right)}{4k^2\xi^2+k_0^2\sinh^2\left(\xi L\right)}. \tag{22}$$

Here T and φ are, respectively, the transmission coefficient (probability) and the phase accumulated by transmitted particles due to the rectangular barrier in the absence of the magnetic field. These magnitudes are given by:

$$T = \left\{1+\frac{\left(k^2+\xi^2\right)^2\sinh^2\left(\xi L\right)}{4k^2\xi^2}\right\}^{-1} \tag{23}$$

and

$$\tan\varphi = \frac{k^2-\xi^2}{2\xi k}\tanh\left(\xi L\right). \tag{24}$$

The total BL time, defined by Eq. (11), and which corresponds to the characteristic time for the spin component along the direction of the original polarization, is then given by:

$$\tau^{\rm BL} = \frac{m}{\hbar\xi}\left\{\left(\frac{\partial\ln T^{1/2}}{\partial\xi}\right)^2+\left(\frac{\partial\varphi}{\partial\xi}\right)^2\right\}^{1/2}. \tag{25}$$

This is the BL traversal time for a rectangular barrier.

It is not difficult to check that when the energy E of an incident particle is well below the barrier height V_0 of an opaque rectangular barrier $\theta_\parallel^2 \gg \theta_\perp^2$ and Büttiker's result (25) is approximately equal to

$$\tau^{\rm BL} \simeq \frac{mL}{\hbar\xi} \tag{26}$$

which is very different from the result of Rybachenko, Eq. (8). It is, however, in exact agreement with the traversal time obtained by Büttiker and Landauer [55] based on the transition from adiabatic to sudden limits for a time–modulated rectangular opaque barrier (see the subsection on the Time-Modulated Barrier Approach).

III. FORMALISM IN TERMS OF GREEN'S FUNCTIONS

Let us now derive a general expression for the Büttiker-Landauer traversal (and reflection) time using the Green's Function (GF) method [56, 57]. We will consider a 1D system with an arbitrary potential $V(y)$ confined to a finite segment $0 < y < L$, as represented in fig. 1. We will call this region "the barrier", and we will assume that scattering in it to be purely elastic. As in the case of a rectangular barrier, we apply a weak magnetic field $\mathbf{B}$ in the z direction and confined to the barrier:

$$\mathbf{B} = B\theta(y)\theta(L-y)\hat{\mathbf{z}} \tag{27}$$

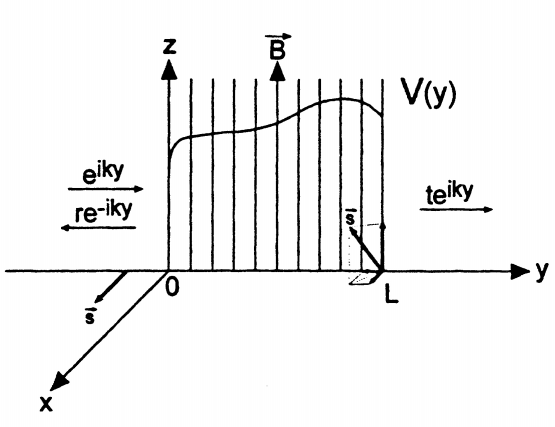

FIG. 3: General potential barrier restricted to the interval $0 < y < L$ with a magnetic field applied.

here $\theta(y)$ is the step function (later *theta* will refer to a completely different function).

If we concentrate in the motion of an electron, with spin $S = 1/2$, we have to consider its two wave functions Ψ_1 and Ψ_2, corresponding to the two spin projections of $+1/2$ and $-1/2$ along the z axis. The column wave function $\widehat{\Psi}(y)$ represents compactly both spin states:

$$\widehat{\Psi}(y) = \begin{pmatrix}\Psi_1\\ \Psi_2\end{pmatrix}. \tag{28}$$

Our electron is incident on the barrier from the left with an energy E and with its spin polarized along the x direction, so its wave function before entering the barrier is given by:

$$\widehat{\Psi}(y) = \begin{pmatrix}1\\ 1\end{pmatrix}\exp(iky). \tag{29}$$

where $k_0 = (2mE)^{1/2}/\hbar$. We are considering a plane wave for the wave function, but our results are valid for any wavepacket provided it is much longer than the size of the barrier L.

In the presence of a magnetic field, Schrödinger equation takes the form:

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dy^2}+V(y)-E\right)\widehat{\Psi}(y) = -\mu\mathbf{B}\ \widehat{\Psi}(y)$$
$$= -\mu B\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\widehat{\Psi}(y). \tag{30}$$

The term on the right–hand side describes the interaction $-\mu\mathbf{B}$; since by assumption the vector $\mathbf{B}$ is directed along the z–axis and the magnetic moment μ is of the form $\mu = 2\mu\mathbf{S}$, where $\mathbf{S}$ is the particle spin vector. We have:

$$\mu\mathbf{B} = 2\mu S_z B = \mu\sigma_z B = \mu B\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}, \tag{31}$$

where σ_z is a Pauli matrix.

The problem is solved by perturbation theory. In the lowest order in B, the spinor $\widehat{\Psi}(L)$ of the electron on the right end of the barrier is given by [56]:

$$\widehat{\Psi}(L) = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \psi(L) + \frac{e\hbar B}{2mc} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \int_0^L \psi(y) G(y, L)\, dy. \tag{32}$$

Here $\psi(y)$ is the solution of the spatial part of the Schrödinger equation in the absence of the magnetic field. This spatial part of the wave function can be written in terms of the GF of the system as:

$$\psi(y) = \exp(iky) - \int_0^L G(y, y') V(y') \exp(iky')\, dy', \tag{33}$$

where $G(y, y')$ is the retarded GF, whose energy dependence is not written explicitly. It should satisfy Dyson's equation:

$$G(y, y') = G_0(y, y') + \int_0^L G_0(y, y'') V(y'') G(y'', y')\, dy'', \tag{34}$$

where $G_0(y, y') = i \left(m/k\hbar^2\right) \exp(ik|y - y'|)$ is the free-electron GF. We can obtain all the relevant properties of the problem in terms of the GF, solution of the previous equation.

A Traversal Time

We will first concentrate on the calculation of the traversal time. The expectation value of the component of the spin along the direction of the magnetic field of the transmitted electron is, up to second order in B:

$$\begin{aligned} \langle S_z \rangle &= \frac{\hbar}{2} \left\langle \widehat{\Psi}(L) \mid \sigma_z \mid \widehat{\Psi}(L) \right\rangle \\ &= -\frac{e\hbar^2 B}{mc} \mathrm{Re} \left[\psi^*(L) \int_0^L \psi(y) G(L, y)\, dy \right] \end{aligned} \tag{35}$$

We want to express the wave function $\psi(y)$ appearing inside the integral in the previous equation in terms of the GF. In order to do so, we take into account the following relationship between the wave function and the GF of a 1D system:

$$\psi(y) = -\frac{i\hbar^2 k}{m} G(0, y). \tag{36}$$

For one-dimensional systems also, we can further simplify the problem by writing the general expression of the GF, $G(y, y')$, in terms of its own expression at coinciding coordinates $y = y'$ [58]:

$$\begin{aligned} &G(y, y') = \\ &[G(y, y) G(y', y')]^{1/2} \exp\left\{ - \int_{\min(y,y')}^{\max(y,y')} \frac{m}{\hbar^2} \frac{dy_1}{G(y_1, y_1)} \right\} = \\ &[G(y, y) G(y', y')]^{1/2} \exp\left[i \left| \theta(y) - \theta(y') \right| \right], \end{aligned} \tag{37}$$

where the phase factor $\theta(y)$, which implicitly depends on energy, is defined as:

$$\theta(y) = \int_0^y \frac{im}{\hbar^2} \frac{dy'}{G(y', y')}. \tag{38}$$

In Appendix B we will use the relation (37) to calculate the transmission coefficient of an electron through a layered system.

Substituting expression (37) for the GF into Eq. (36) and making use of the relation between the wave function and the GF, Eq. (36), one finds the spin component along the direction of the magnetic field:

$$\langle S_z \rangle = \frac{e\hbar^2 B}{mc} |\psi(L)|^2 \,\mathrm{Re} \int_0^L G(y, y)\, dy, \tag{39}$$

A similar procedure for the spin component along the y and x directions leads to

$$\langle S_y \rangle = -\frac{e\hbar^2 B}{mc} |\psi(L)|^2 \,\mathrm{Im} \int_0^L G(y, y)\, dy. \tag{40}$$

and

$$\langle S_x \rangle = \frac{\hbar}{2} |\psi(L)|^2 \left(1 - \frac{1}{2} \left| \frac{2e\hbar B}{mc} \int_0^L G(y, y)\, dy \right|^2 \right). \tag{41}$$

Büttiker–Landauer characteristic traversal times for the z and y directions are proportional to the corresponding spin components, Eqs. (19) and (18), and we finally arrive at:

$$\begin{aligned} \tau_z^{\mathrm{BL}} &= \hbar \,\mathrm{Re} \int_0^L G(y, y)\, dy, \\ \tau_y^{\mathrm{BL}} &= \hbar \,\mathrm{Im} \int_0^L G(y, y)\, dy, \end{aligned} \tag{42}$$

So, the Büttiker–Landauer traversal time, Eq. (11), is given by:

$$\tau^{\mathrm{BL}} = \hbar \left| \int_0^L G(y, y)\, dy \right|. \tag{43}$$

Instead of defining the modulus of τ_z^{BL} and τ_z^{BL} as the central magnitude of the problem, we prefer to define a complex traversal time τ as:

$$\tau = \tau_z^{\mathrm{BL}} + i\tau_y^{\mathrm{BL}} = \hbar \int_0^L G(y, y)\, dy. \tag{44}$$

As we will see, other approaches also get a complex time. All we are saying is that the two characteristic times of the problem can be written in a compact form as the real an imaginary parts of a single well-defined magnitude. Besides, these two time components may be separately relevant to different experimental results, and do not have to necessarily enter into the problem through the modulus, Eq. (43). We will come back to this question in the next section.

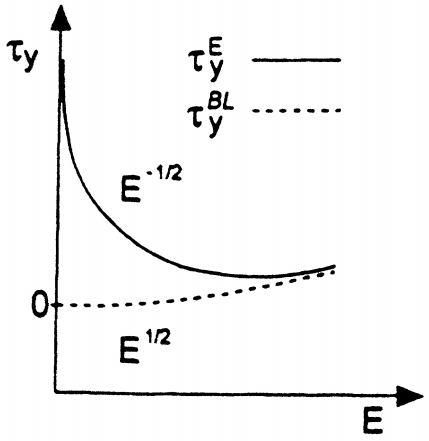

FIG. 4: Traversal time for a rectangular barrier according to expressions (47) and (80).

1 *Expression in terms of transmission and reflection amplitudes*

The final result, Eq. (43) or Eq. (44), only depends on the integral of the GF at coinciding coordinates. For practical purposes and in order to compare this result with those of other approaches, it is interesting to rewrite it in terms of the transmission t and reflection r amplitudes, or, alternatively, in terms of the transmission T and reflection $R = 1 - T$ probabilities and the phases φ and $\varphi \pm \varphi_a$ of the scattering-matrix elements $s_{\alpha\beta}$

$$s(E) = \begin{pmatrix} r & t \\ t & r' \end{pmatrix} \tag{45}$$

$$= \begin{pmatrix} -i\sqrt{R}\exp(i\varphi + i\varphi_a) & \sqrt{T}\exp(i\varphi) \\ \sqrt{T}\exp(i\varphi) & -i\sqrt{R}\exp(i\varphi - i\varphi_a) \end{pmatrix} \tag{46}$$

This scattering matrix is assumed to be symmetric, which holds in the absence of a magnetic field. φ_a is an extra phase accumulated by reflected particles incident from the left, with respect to transmitted particles. Reflected particles incident from the right accumulate the opposite phase. For a spatially symmetric barrier $V((L/2)+y) = V((L/2)-y)$ the phase asymmetry φ_a vanishes and one has additionally $r = r'$.

The integral of the GF at coinciding coordinates can be calculated quite generally in a finite region in terms of t and r (Aronov *et al.* [58], Gasparian *et al.* [57]). In appendix C we show how to perform this calculation. Making use of the Eqs. (C4), (C7) and (C8), it is straightforward to show that the spatial integral, over the length of the barrier, of the GF at coinciding coordinates can be expressed in terms of partial derivatives with respect to energy E:

$$\boxed{\tau = \hbar \int_0^L G(y,y)\, dy = \hbar \left\{ \frac{\partial \ln t}{\partial E} + \frac{1}{4E}(r + r') \right\}} \tag{47}$$

This is a general expression, independent of the model considered.

For an arbitrary 1D potential profile, the two components of the tunneling time τ_z and τ_y, can be written in general as the real and imaginary parts of Eq. (47). Using the explicit expression of the matrix element of the scattering matrix, Eq. (45), we find

$$\tau_z^{\mathrm{BL}} \equiv \hbar\, \mathrm{Re} \int_0^L G(y,y)\, dy \tag{48}$$

$$= \hbar \left(\frac{d \ln T}{2dE} + \frac{\sqrt{R}}{2E} \sin(\varphi)\cos(\varphi_a) \right), \tag{49}$$

$$\tau_y^{\mathrm{BL}} \equiv \hbar\, \mathrm{Im} \int_0^L G(y,y)\, dy \tag{50}$$

$$= \hbar \left(\frac{d\varphi}{dE} - \frac{\sqrt{R}}{2E} \cos(\varphi)\cos(\varphi_a) \right) \tag{51}$$

The term proportional to $\partial \ln t/\partial E$ in Eq. (47), or equivalently the first term on the RHS of Eqs. (48) and (50), mainly contains information about the region of the barrier. Most of the information about the boundary is provided by the reflection amplitudes r and r', and is on the order of the wavelength λ over the length of the system L, i.e. $0(\lambda/L)$. Thus, it becomes important for low energies and/or short systems. This term can be neglected in the semiclassical WKB case and, of course, when r (and so r') is negligible, e.g., in the resonant case, when the influence of the boundaries is negligible. Certain approaches share this feature of only obtaining the contribution to the time proportional to an energy derivative, missing the terms proportional to the reflection amplitudes. We will discuss this point in more detail later on. The same type of problem arises when calculating densities of states or partial densities of states [59].

2 *Properties of the traversal time*

The integral of the GF at coinciding coordinates, and so the components of the traversal time, can be related to the density of states and the resistance. It is well known that the imaginary part of $G(y,y)$ is proportional to the local density of states at the corresponding energy. So, τ_y^{BL} can also be written in terms of the average density of states of the electron in the system per unit energy and per unit length $\nu_L(E)$:

$$\tau_y^{\mathrm{BL}} = \pi\hbar L \nu_L(E). \tag{52}$$

Landauer's conductance for a 1D structure coupled to two perfect leads $G(E)$ is related to the transmission coefficient T by the expression [60]

$$G(E) = \frac{2e^2}{\hbar} T \tag{53}$$

Substituting this result in Eq. (48) we obtain the following expression for the characteristic time $\tau_z^{\rm BL}$:

$$\tau_z^{\rm BL} = \hbar \left(\frac{d \ln G(E)}{2dE} + \frac{\sqrt{1-\hbar/2e^2G(E)}}{2E} \sin(\varphi)\cos(\varphi_a) \right) \tag{54}$$

Thouless has shown [61] the existence of a dispersion relation between the localization length and the density of states. This relationship can be expressed (Gasparian *et al.*, [62]) in the form of a linear dispersion relation between the real part, $\mathrm{Re}\ln t$, and the imaginary part, $\mathrm{Im}\ln t$, of the transmission amplitude. The self–averaging property of $\tau_z^{\rm BL}$ and of $\tau_y^{\rm BL}$ is therefore an immediate consequence of self-averaging of the localization length and of the density of states [62]. If one calculates the transmission time through a barrier by dividing the barrier arbitrarily into two parts, the total tunneling time $\tau^{\rm BL}$, given by Eq. (43), is not the sum of the individual transmission times, as one could expect. On the contrary, one can easily deduce from Eqs. (48) and (50) that τ_z and τ_y are additive, in the sense that

$$\begin{aligned} \tau_z^{\rm BL}(0,L) &= \hbar\,\mathrm{Re}\int_0^L G(y,y)\ dy \qquad (55)\\ &= \hbar \mathrm{Re}\left[\int_0^y G(y,y)\ dy + \int_y^L G(y,y)\,dy\right] \\ &= \tau_z^{\rm BL}(0,y) + \tau_z^{\rm BL}(y,L) \\ \tau_y^{\rm BL}(0,L) &= \hbar\,\mathrm{Im}\int_0^L G(y,y)\ dy \qquad (56)\\ &= \hbar \mathrm{Im}\left[\int_0^y G(y,y)\,dy + \int_y^L G(y,y)\,dy\right] \\ &= \tau_y^{\rm BL}(0,y) + \tau_y^{\rm BL}(y,L) \end{aligned}$$

This property has also been pointed out by Leavens and Aers [63] when they discussed the local version of the Larmor clock with an arbitrary barrier potential and a localized magnetic field inside the barrier. It is a consequence of the fact that for an infinitesimal B the interference between the effects the of magnetic field in the separate regions $[0;y]$ and $[y;L]$ is of higher order than linear and does not contribute to the local times (Leavens and Aers [63]). Mathematically speaking, we say that the BL time, Eq. (43), adds as the absolute value of complex additive numbers, and so it is not additive.

B Reflection Time

For reflected particles we can proceed in the same way as for transmitted particles. The change in orientation of the spin of reflected waves and so the reflection time $\tau_{\rm R}$ from an arbitrary 1D barrier can be calculated in the same way as we have done for transmitted waves. We will use the subindex R to indicate that the magnitude corresponds to reflection, and we understand that similar magnitudes related to transmission will have no subindex. Proceeding as above, we find for the expectation values of the spin components of the reflected wave:

$$\begin{aligned} \langle S_z\rangle_{\rm R} &= \frac{\hbar}{2}\left\langle \left(\widehat{\Psi}(0)-1\right) \mid \sigma_z \mid \left(\widehat{\Psi}(0)-1\right)\right\rangle \qquad (57)\\ &= \frac{e\hbar^2 B}{mc}\,|\psi^*(0)-1\ |^2\,\mathrm{Re}\int_0^L \psi(y)G(0,y)\,dy \end{aligned}$$

$$\langle S_y\rangle_{\rm R} = -\frac{e\hbar^2 B}{mc}\ |\psi^*(0)-1\,|^2\,\mathrm{Im}\int_0^L \psi(y)G(0,y)\,dy \tag{58}$$

and

$$\langle S_x\rangle_{\rm R} = \tag{59}$$
$$\frac{\hbar}{2}\,|\psi^*(0)-1|^2\left(1-\frac{1}{2}\left|\frac{2e\hbar B}{mc}\int_0^L \psi(y)G(0,y)\,dy\right|^2\right)$$

Following Büttiker [45] we can again define three new characteristic times, $\tau_{z,\rm R}^{\rm BL}$, $\tau_{y,\rm R}^{\rm BL}$ and $\tau_{x,\rm R}^{\rm BL}$, each of them associated with a component of the spin through the expressions

$$\lim_{\omega_{\rm L}\to 0}\langle S_z\rangle_{\rm R} = \frac{\hbar}{2}\omega_{\rm L}\tau_{z,\rm R}^{\rm BL}, \tag{60}$$

$$\lim_{\omega_{\rm L}\to 0}\langle S_y\rangle_{\rm R} = -\frac{\hbar}{2}\,\omega_{\rm L}\tau_{y,\rm R}^{\rm BL}, \tag{61}$$

$$\lim_{\omega_{\rm L}\to 0}\langle S_x\rangle_{\rm R} = \frac{\hbar}{2}\left[1-\frac{\omega_{\rm L}^2\left(\tau_{x,\rm R}^{\rm BL}\right)^2}{2}\right] \tag{62}$$

Only two of these times are independent. Invoking Eqs. (57–59) and the relationship (36) between the wave function and the GF of a one-dimensional system we arrive at:

$$\tau_{y,\rm R}^{\rm BL} = \hbar\,\mathrm{Im}\frac{1+r}{r}\ e^{-i2\theta(0)}\int_0^L G(y,y)e^{i2\theta(y)}\,dy \tag{63}$$

$$\tau_{z,\rm R}^{\rm BL} = \hbar\,\mathrm{Re}\ \frac{1+r}{r}\ e^{-i2\theta(0)}\int_0^L G(y,y)e^{i2\theta(y)}\,dy \tag{64}$$

where $\theta(y)$ is the phase function given by Eq. (38). The characteristic times $\tau_{y,\rm R}^{\rm BL}$ and $\tau_{z,\rm R}^{\rm BL}$ are the real and imaginary components, respectively, of a complex quantity. This quantity is proportional to a new integral of the GF at coinciding coordinates, which in this case involves the phase function also.

The previous integral can be expressed in terms of the transmission and reflection amplitudes. In appendix C we show how to perform this integral exactly. Making use of the integral relations (C5) and (C11) of the GF at

coinciding coordinates we finally obtain for the reflection times (Gasparian [64]):

$$\tau_{y,\mathrm{R}}^{\mathrm{BL}} = \hbar\,\mathrm{Im}\,\left\{\frac{\partial \ln r}{\partial E} - \frac{1}{4Er}\left(1-r^2-t^2\right)\right\} \tag{65}$$

and

$$\tau_{z,\mathrm{R}}^{\mathrm{BL}} = \hbar\,\mathrm{Re}\,\left\{\frac{\partial \ln r}{\partial E} - \frac{1}{4Er}\left(1-r^2-t^2\right)\right\} \tag{66}$$

These equations are correct for any arbitrary 1D potential $V(y)$. These two characteristic reflection times $\tau_{y,\mathrm{R}}^{\mathrm{BL}}$ and $\tau_{z,\mathrm{R}}^{\mathrm{BL}}$ can be written as the complex reflection time τ_{R}, in analogy with the complex traversal time τ, Eq. (44):

$$\boxed{\tau_{\mathrm{R}} = \tau_{z,\mathrm{R}}^{\mathrm{BL}} + i\tau_{y,\mathrm{R}}^{\mathrm{BL}} \equiv \hbar\left\{\frac{\partial \ln r}{\partial E} - \frac{1}{4Er}\left(1-r^2-t^2\right)\right\}} \tag{67}$$

This is again a general equation, independent of the model used.

We note that for an arbitrary symmetric potential, $V((L/2)+y) = V((L/2)-y)$, the total phases accumulated in a transmission and in a reflection event are the same, as can be deduced from the form of the scattering matrix elements, Eq. (45)), and so the characteristic times for transmission and reflection corresponding to the direction of propagation are equal

$$\tau_{y}^{\mathrm{BL}} = \tau_{y,\mathrm{R}}^{\mathrm{BL}} \tag{68}$$

as it immediately follows from Eqs. (50) and (65) (see also the review article by Hauge and Støvneng [4]). For the special case of a rectangular barrier, Eq. (68) was first found by Büttiker [45]. Comparison of the Eqs. (50) and (65) shows that for an asymmetric barrier Eq. (68) breaks down (Leavens and Aers [65]).

As a consequence of the conservation of angular momentum we can write the following identity between the characteristic times for transmission and reflection corresponding to the direction of the magnetic field (Büttiker [45], Sokolovski and Baskin [66])

$$R\tau_{z,\mathrm{R}}^{\mathrm{BL}} + T\tau_{z}^{\mathrm{BL}} = 0 \tag{69}$$

which can be checked directly using Eqs. (48) and (66).

IV. OTHER APPROACHES

We now review other approaches to the problem of the traversal and reflection times. We would like to show that most results, obtained from very different points of view, are almost compatible and coincide with Eq. (47) for the traversal time and with Eq. (67) for the reflection time. Often, these approaches only obtain the contributions to the time proportional to the energy derivative of the logarithm of the transmission amplitude.

We start with the oscillatory incident amplitude and with the time-modulated barrier approaches. Then we review the Feynman path-integral approach, where the idea of a complex time arises more naturally. And we finish with the kinetic approach, which is very convenient to study finite size effects and so the standard errors inherent to the problem.

A Oscillatory incident amplitude

Let us now assume an incident wave of oscillatory amplitude interacting with a time–independent potential, and let us study the shape distortion of the transmitted wave by the barrier. This method was proposed by Büttiker and Landauer [67, 68] and analyzed by Leavens and Aers [65] and Martin and Landauer [69]. The incident wave consists of two interfering plane waves:

$$\begin{aligned}\Psi(y,t) &= \exp\left\{i\left[ky - \frac{Et}{\hbar}\right]\right\} \\ &+ \exp\left\{i\left[(k+\Delta k)y - \frac{(E+\Delta E)t}{\hbar}\right]\right\} \\ &= 2\exp\left\{i\left[(k+\Delta k/2)y - \frac{(E+\Delta E/2)t}{\hbar}\right]\right\} \\ &\cos\left(\frac{\Delta k y}{2} - \frac{\Delta E t}{2\hbar}\right)\end{aligned} \tag{70}$$

The energy difference between the two plane waves characterizes the oscillations in amplitude of the incident wave. In the region to the right of the barrier we have the sum of two transmitted plane waves which can be written in the form

$$\begin{aligned}\Psi(y,t) &= t(E)\left\{i\left[ky - \frac{Et}{\hbar}\right]\right\} + \\ &t(E+\Delta E)\exp\left\{i\left[(k+\Delta k)y - \frac{(E+\Delta E)t}{\hbar}\right]\right\}.\end{aligned} \tag{71}$$

It is clear that the shape distortion produced by the barrier on the transmitted wave will strongly depend on ΔE. If ΔE is small, the incident wave is modulated very slowly and in that case the transmitted wave (71) will reproduce the incident wave (70), in the sense that the destructive and constructive interferences will occur at the same time for both of them. As we increase ΔE, $t(E)$ and $t(E+\Delta E)$ will increasingly differ and the transmitted wave (71) will no longer reproduce the incident wave. We can assume that appreciable shape distortion will take place when a characteristic time delay, or dispersion in transit time, becomes comparable or larger than the modulation period [67, 68]. Thus we define a new traversal time τ as $\hbar/\Delta E$, where ΔE is the energy difference which establishes the onset of significant distortion of the transmitted wave, i.e., the energy such that $\Delta E\,|d\alpha(E)/dE| \approx 1$.

The analysis of this approach based on the WKB approximation lead Büttiker and Landauer [67] to the following results. For $E < V(y)$ the phase of the transmission amplitude is of secondary importance as compare with the exponential decay of the modulus of $t(E)$. We can write the transmission amplitude in the form

$$t_{\rm WKB}(E) = \exp\left[-\int_{y_1}^{y_2} \xi(y)\, dy\right] \tag{72}$$

where ξ is the inverse decay length, given by Eq. (9), and y_1 and y_2 are the classical turning points. From this expression of the transmission amplitude, Büttiker and Landauer obtained for the traversal time for tunneling

$$\tau_{\rm WKB}(E) = \frac{m}{\hbar}\left[-\int_{y_1}^{y_2} \frac{dy}{\xi(y)}\right] \tag{73}$$

In the case of transmission over a barrier, when $E > V(y)$, the energy dependence of $t(E)$ comes primarily from the dependence of the phase ($|t(E)| = 1$), and then we can assume that $t(E)$ is of the form

$$t_{\rm WKB}(E) = \exp\left[-i\int_0^L K(y)dy\right] \tag{74}$$

with $K(y) = i\xi(y)$. For this case, in which the phase dominates we have

$$\tau_{\rm WKB}(E) = \frac{m}{\hbar}\left[\int_0^L \frac{dy}{K(y)}\right] \tag{75}$$

It is easy to check that for a rectangular barrier the traversal time $\tau_{\rm WKB}$ is equal to $mL/\hbar\xi$ for energies bellow the barrier height and equal to $mL/\hbar K$ for energies above the barrier. As it was shown by Martin and Landauer [69] the general analysis of this two interfering incident waves approach yields characteristic times that depend on energy derivatives of the transmission coefficient

$$\tau = \hbar\left|t_E^{-1}\right|\left|\frac{dt_E}{dE}\right| = \hbar\left\{\left(\frac{d\varphi}{dE}\right)^2 + \left(\frac{d\ln T}{dE}\right)^2\right\}^{1/2}. \tag{76}$$

As in Büttiker and Landauer approach to the Larmor clock, the time is equal to the square root of the sum of the squares of two characteristic times, one involving energy derivatives of the phase and the other energy derivatives of the logarithm of the modulus of the transmission amplitude. The same result for the traversal time is also obtained in the modulated barrier approach (Martin and Landauer [69]).

It is interesting to note that this oscillatory amplitude approach without resort to the WKB approximation lead Leavens and Aers [65] to complex times. Let us write the transmission amplitude as:

$$t(E) = \exp\left[i\beta(E)\right] \tag{77}$$

where $\beta(E)$ is in general complex. For sufficiently small ΔE we may expand $t(E+\Delta E)$ to lowest order in ΔE

$$\begin{aligned} t(E+\Delta E) &\cong \exp\left[i\left(\beta(E) + \Delta E\frac{d\beta(E)}{dE}\right)\right] \\ &= t(E)\exp\left[i\Delta E\frac{d\beta(E)}{dE}\right]. \end{aligned} \tag{78}$$

This expression should be substituted in Eq. (71) for the transmitted packet. For sufficiently small ΔE the difference in exponents of the two components of the transmitted wave at $y = L$ and $t = \Delta t$ is greater than that of the two components of the incident wave at $y = 0$ and $t = 0$ by an amount

$$\begin{aligned} & i\left[\Delta kL - \frac{\Delta E}{\hbar\Delta k}\left(\Delta t - \hbar\frac{d\beta(E)}{dE}\right)\right] \\ & \cong i\Delta k\left[L - v(k)\left(\Delta t - \hbar\frac{d\beta(E)}{dE}\right)\right] \end{aligned} \tag{79}$$

with $v(k) \equiv \hbar^{-1}dE/dk = \hbar k/m$ being the group velocity. In the absence of the potential barrier the traversal time associated with the propagation of the wavepacket from $y = 0$ to $y = L$ is the value of Δt for which $L - v(k)\Delta t = 0$, i.e., $\tau = L/v(k)$. Formally, in the presence of the potential, Leavens and Aers [65] obtained from Eq. (79) the complex barrier interaction "time"

$$\tau^E = \frac{L}{v(k)} + \hbar\frac{d\beta(E)}{dE} \equiv -i\hbar\frac{\partial \ln t}{\partial E} \tag{80}$$

This final answer for the time is just proportional to $\partial \ln t/\partial E$, and so is correct for infinitely large systems only ($L \gg \lambda$). The difference between this expression for the traversal time and our general expression (47) is the term proportional to the reflection amplitude, which cannot be obtained with this type of approach.

We can deduce explicit expressions for all these times, and so see clearly the difference between Eq. (80) and Eq. (47), obtained with the GF formalism, for the special case of a rectangular barrier. Let us associate the real and imaginary components of this complex time, Eq. (80), with the previous characteristic times for the y and z components, and let us denote them as τ_y^E and τ_z^E. The explicit expressions for the two components of the traversal time τ_y^E and τ_z^E for this special case of a constant potential can be written, using the well known expressions (23) and (24), in the form [65]:

$$\begin{aligned} \tau_z^E &= -\hbar\frac{\partial \ln T^{1/2}}{\partial E} \\ &= \frac{mk_0^4}{2\hbar\xi^2k^2}\frac{2(\xi^2-k^2)\sinh^2(\xi L) + k^2\xi L\sinh(2\xi L)}{4k^2\xi^2 + k_0^2\sinh^2(\xi L)} \end{aligned} \tag{81}$$

$$\tau_y^E = \hbar\frac{\partial\varphi}{\partial E} = \frac{m}{\hbar k\xi}\frac{2\xi Lk^2(\xi^2-k^2) + k_0^4\sinh(2\xi L)}{4k^2\xi^2 + k_0^2\sinh^2(\xi L)} \tag{82}$$

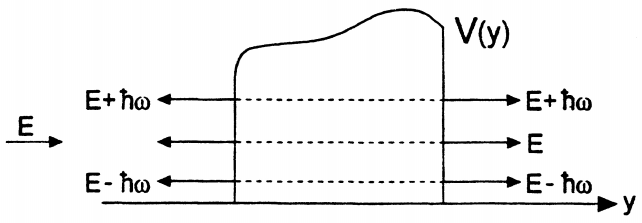

FIG. 5: For an oscillating barrier besides a main transmission and reflection component at the initial energy E there are two lateral components at energies $E \pm \hbar\omega$.

After an obvious change of notation, it is easy to check that the times τ_y^E and τ_z^E are related to the exact results $\tau_y^{\rm BL}$ and $\tau_z^{\rm BL}$ through:

$$\tau_y^E = \tau_y^{\rm BL} + \frac{1}{2E}{\rm Im}\, r,$$
$$-\tau_z^E = \tau_z^{\rm BL} + \frac{1}{2E}{\rm Re}\, r. \qquad (83)$$

where $\tau_z^{\rm BL}$ and $\tau_y^{\rm BL}$ are given by Eqs. (21) and (22). Fig.5 compares τ_z^E with $\tau_z^{\rm BL}$, and also τ_y^E with $\tau_y^{\rm BL}$ for a rectangular barrier. It can be seen that even for an opaque barrier ($\xi L \gg 1$) the differences between these times can be very significant. This is particularly so at very small energy E where $\tau_y^{\rm BL}$ goes to zero as $E^{1/2}$, while τ_y^E diverges as $E^{-1/2}$, and, at the same time, $\tau_z^{\rm BL}$ is approximately equal to 0, while τ_z^E diverges as E^{-1}.

It is clear that the oscillatory amplitude approach in general does not give the same answer as the GF formalism, based on the Larmor clock approach. As the difference between the corresponding tunneling times is proportional to the amplitude of reflection, we concluded that it arises from boundary effects [57].

B Time–Modulated Barrier

The time–modulated barrier approach, which again can be used to measure the traversal time, was introduced by Büttiker and Landauer [55] (see also Refs. [67, 70]). Its basic idea is simple and can be explained as follows.

Let us add to the static barrier potential which we discussed before a time dependent potential which is zero everywhere except in the region of interest. So the 1D potential can now be written in the form

$$V(y,t) = V(y) + V_1 \cos(\omega t) \qquad (84)$$

where V_1 is the amplitude of the small modulation added, and ω its corresponding frequency. For the sake of simplicity it is more convenient in this approach to consider the barrier restricted to the region $-L/2 < y < L/2$.

Suppose that there is a characteristic time τ during which the particle interacts with the barrier. If the period of the modulation $T = 2\pi/\omega$ is long compared to the time τ, then the particle sees an effectively static barrier during its traversal. In the opposite extreme, i.e., for slowly tunneling electrons, for which $\omega\tau > 1$, the barrier oscillates many times during the period of traversal of the electron. There is thus a crossover from a low–frequency behavior to a high–frequency behavior, and we expect to occur two distinct types of electron–barrier interactions, depending on the value of $\omega\tau$ as compared with unity.

In this section we will use a rectangular barrier extensively, for illustrative purposes, but in principle all the results can be generalized to an arbitrary potential barrier by considering the adiabatic limit, $\omega \to 0$, of this inelastic scattering process [71]. The Hamiltonian for the time–modulated rectangular barrier in the scattering region is

$$H = -\frac{\hbar}{2m}\frac{d^2}{dy^2} + V_0 + V_1\cos(\omega t) \equiv H_0 + V_1\cos(\omega t) \quad (85)$$

As it is well known from the time–dependent perturbation theory (Landau and Lifshits [72]), incident particles with energy E, interacting with the perturbation $V_1\cos(\omega t)$, will emit or absorb modulation quanta $\hbar\omega$. In first–order corrections to the time–independent case, this means that inside the barrier, for $|y| > L/2$, the reflected and transmitted waves, used to represent the tunneling electrons, we will now have a main feature at the initial energy E and also side bands at the energies $E+\hbar\omega$ and $E-\hbar\omega$, as it is schematically represented in fig.5. Taking V_1 as a perturbation the two independent eigensolutions of the corresponding time–dependent Schrödinger equation, within the rectangular barrier, can be written as (Landau and Lifshits [72])

$$\Psi_{\rm bar}(y,t;E) = \varphi_E(y)\exp\left\{-\frac{iEt}{h}\right\}\exp\left\{-\frac{iV_1}{\hbar\omega}\sin\omega t\right\}. \qquad (86)$$

Here $\varphi_E = e^{\pm\xi y}$ is a wave function solution of the time–independent problem $H_0\varphi_E = E\varphi_E$, with the simpler Hamiltonian H_0.

As it was shown by Büttiker and Landauer [55], the next stage to find the solution for the oscillating rectangular barrier is to match Eq. (86) with the corresponding solutions at the same energy outside the scattering region. For an electron of energy E impinging on the scattering region, there will be reflected and transmitted waves at the three energies E, $E+\hbar\omega$ and $E-\hbar\omega$. So, if the electron is coming from the left, its wave function in the region to the left of the barrier, $y < -L/2$, will be of the form

$$\Psi_{\rm inc+ref} = (e^{ik(y+L/2)} + re^{-ik(y+L/2)})e^{-iEt/\hbar} + r_+e^{-ik_+(y+L/2)}e^{-i(E+\hbar\omega)t/\hbar} + r_-e^{-ik_-(y+L/2)}e^{-i(E-\hbar\omega)t/\hbar} \qquad (87)$$

where $k_\pm$ are the wavevectors corresponding to the side energy bands, defined as $k_\pm = (2m/\hbar^2)^{1/2}(E \pm \hbar\omega)^{1/2}$.

Equation (87) represents an incident plane wave of unit amplitude and three reflected waves, one of amplitude r at the incident energy and two of amplitudes $r_\pm$ at energies $E \pm \hbar\omega$. To the right of the barrier ($y > L/2$), we have for the transmitted wave

$$\Psi_{\rm tra} = te^{ik(y-L/2)}e^{-iEt/\hbar} + t_+e^{ik_+(y-L/2)}e^{-i(E+\hbar\omega)t/\hbar} + t_-e^{ik_-(y-L/2)}e^{-i(E-\hbar\omega)t/\hbar} \quad (88)$$

where t is the transmission amplitude at the energy of the incident wave and $t_\pm$ are the transmission amplitudes of the sidebands.

In the barrier, for an infinitesimal amplitude of the time–dependent potential, $V_1 \ll \hbar\omega$, we can expand (86) to lowest order in V_1 and represent the wave function in the form:

$$\begin{aligned}\Psi_{\rm bar} = &\left[Be^{\xi y} + Ce^{-\xi y}\right]e^{-iEt/\hbar} \\ &\left[1 + \frac{V_1}{2\hbar\omega}e^{-i\omega t} - \frac{V_1}{2\hbar\omega}e^{i\omega t}\right] \\ &+ \left[B_+e^{\xi+y} + C_+e^{-\xi+y}\right]e^{-i(E+\hbar\omega)t/\hbar} \\ &+ \left[B_-e^{\xi-y} + C_-e^{-\xi-y}\right]e^{-i(E-\hbar\omega)t/\hbar}\end{aligned} \quad (89)$$

$\xi_\pm$ are the inverse decay lengths for the sidebands, defined as $\xi_\pm = (2m/\hbar^2)^{1/2}\,(V_0 - E \mp \hbar\omega)^{1/2}$. The coefficients r, $r_\pm$, B, $B_\pm$, C, $C_\pm$, t, and $t_\pm$ are determined by matching the wave functions and their derivatives at $y = -L/2$ and at $y = L/2$ in the usual manner. Note that the matching conditions must hold for all times; therefore, we have to match each time Fourier component separately. r and t play the role of the static reflection and transmission amplitudes, respectively. Using the standard matching relations it is straightforward to show that for an almost completely reflecting barrier in the opaque limit, $\xi L \gg 1$, the coefficient t of the static barrier is given by the standard expression (Landau and Lifshits [72])

$$t = \frac{4k\xi}{k_0^2}e^{-\xi L}\exp\left\{-i\arctan\left[\frac{\xi^2 - k^2}{2k\xi}\right]\right\} \exp\left\{i\left[y - kL - \frac{Et}{\hbar}\right]\right\} \quad (90)$$

For the transmitted waves at the frequencies $(E/\hbar) \pm \omega$, Büttiker and Landauer found that their transmission coefficients are

$$t_\pm = \mp t\,\frac{V_1}{2\hbar\omega}\,(e^{\pm\omega\tau} - 1) \exp\left\{i\left[k_\pm \mp \frac{m\omega L}{2\hbar} - \frac{(E \pm \hbar\omega)t}{\hbar}\right]\right\}. \quad (91)$$

$\tau = mL/\hbar\xi$ is the time it would take a particle with the velocity $v = \hbar\xi/m$ to traverse the opaque rectangular barrier. To obtain Eq. (91) it was additionally assumed that $\hbar\omega \ll E$, so that the wavevectors of the sidebands are approximately equal to $k_\pm \cong k \pm m\omega/\hbar k$, and also that $\hbar\omega \ll V_0 - E$, so that the decay lengths satisfy $\xi_\pm = \xi \mp m\omega/\hbar\xi$.

Note that for opaque barriers the traversal time $\tau^{\rm BL}$ obtained in the Larmor clock approach, Eq. (26), coincides with the expression considered in the previous equation, $\tau = mL/\hbar\xi$. The classical time that one would obtain in the WKB limit at energies below the peak of the barrier is given by the integral

$$\tau = \int_{y_1}^{y_2}\frac{m}{\hbar\xi(y)}dy = \int_{y_1}^{y_2}\left\{\frac{m}{2\,(V_0(y) - E)}\right\}^{1/2}dy \quad (92)$$

where y_1 and y_2 are the classical turning points. This result also reduces to the value appearing in Eq. (91) for the case of a rectangular barrier, when $V_0(y)$ is constant.

The probability of transmission at the sideband energies, determined from Eq. (91), is

$$T_\pm = |t_\pm|^2 = \left(\frac{V_1}{2\hbar\omega}\right)^2(e^{\pm\omega\tau} - 1)^2T \quad (93)$$

where T is the transmission coefficient for the static barrier, given by Eq. (23). For small frequencies, so that $\omega\tau \ll 1$, the probabilities of transmission for the upper and lower sidebands obtained from Eq. (93) are the same and equal to

$$T_\pm = \left(\frac{V_1\tau}{2\hbar}\right)^2T. \quad (94)$$

Remember that τ is the approximate expression for the Büttiker-Landauer time for an opaque barrier, given by Eq. (26).

At high frequencies, the upper sideband is exponentially enhanced, while the lower sideband is exponentially suppressed. So for an opaque barrier we do indeed have a rather well defined crossover between tunneling at high frequencies and tunneling at low frequencies, with the characteristic time corresponding to the value given by Eq. (26). This characteristic crossover time is the same one appearing in the expression of the transmission coefficients of the sidebands in the adiabatic limit.

1 *General barrier*

Let us briefly discuss the results of the general oscillating barrier problem following the papers of Hauge and Støvneng [4] and [71]. It was shown that in the adiabatic limit, $\omega \to 0$, the expression for the transmission coefficients for the sidebands, Eq. (93), can be generalized in the form:

$$T_\pm = |t_\pm|^2 \to \left(\frac{V_1\left|\tau^{\overline{V}}\right|}{2\hbar}\right)^2\left|t(E,\overline{V})\right|^2 \quad (95)$$

where $|t|^2 = T$ and we have written explicitly the E and $\overline{V}$ dependence of the transmission amplitude t. $\overline{V}$ is the

average value of the barrier potential in the scattering region, i.e.

$$\overline{V} \equiv \frac{1}{L}\int_{-L/2}^{L/2} V(y)dy. \tag{96}$$

$\tau^{\overline{V}}$ is a complex quantity, with the dimensions of time, defined as:

$$\tau^{\overline{V}} = i\hbar \frac{\partial \ln t(E,\overline{V})}{\partial \overline{V}} \tag{97}$$

This quantity characterizes the crossover from the adiabatic to the high frequency limits, and we define it as the traversal time in the time–modulated barrier approach.

The corresponding definition of the reflection time appeals to the adiabatic limit of the reflected sidebands. Their reflection coefficients $R_\pm = |r_\pm|^2$ tend in the adiabatic limit to a expression that can be written as

$$|r_\pm|^2 \to \left(\frac{V_1\left|\tau_{\rm R}^{\overline{V}}\right|}{2\hbar}\right)^2 \left|r(E,\overline{V})\right|^2 \tag{98}$$

where $|r|^2 = R$ is the static reflection coefficient. Again, we have explicitly written the E and $\overline{V}$ dependence of the reflection amplitude r. $\tau_{\rm R}^{\overline{V}}$ is a new complex quantity, playing the role of a reflection time, defined as:

$$\tau_{\rm R}^{\overline{V}} = i\hbar \frac{\partial \ln r(E,\overline{V})}{\partial \overline{V}} \tag{99}$$

As shown in Appendix C, Eqs. (97) and (99), corresponding to the traversal and reflection times in the time–modulated approach, are equivalent to Eqs. (47) and (67), obtained with the GF formalism for the Larmor clock approach. The derivative with respect to the average height of the potential can be written in terms of partial derivatives with respect to energy E (Gasparian *et al.* [57]). Thus the complex times $\tau^{\overline{V}}$ and $\tau_{\rm R}^{\overline{V}}$ are related to the real quantities $\tau_z^{\rm BL}$, $\tau_y^{\rm BL}$, $\tau_{y,{\rm R}}^{\rm BL}$ and $\tau_{z,{\rm R}}^{\rm BL}$ (see Eqs.(48), (50), (65) and (66), respectively) and therefore the BL traversal time can be formally written in the form:

$$\tau^{\rm BL} \equiv \hbar \left|\frac{\partial \ln t(E,\overline{V})}{\partial \overline{V}}\right|. \tag{100}$$

It is still not so clear how this time, which was obtained from an analysis of the time–modulated barrier and which is valid for an arbitrary shaped potential $V(y)$, whose average is $\overline{V}$, can be justified as a traversal time for a general barrier (Jauho and Jonson [73]). In any case note that Eq. (100) for an opaque barrier leads us to Eq. (26), which was obtained by Büttiker's analysis of the Larmor clock [45].

The BL reflection time can be defined as in Eq. (100), but replacing $t(E,\overline{V})$ by $r(E,\overline{V})$.

C Complex Time

Although common sense dictates us that the tunneling time must be a real time and that there are no clocks that measure a complex time, nevertheless the concept of complex time in the theory of the traversal time problem of electrons aroused in many approaches (see Martin [74], and references therein). The optical analog of the Larmor clock for classical electromagnetic waves based on Faraday–effect lead us also to a complex time (Gasparian *et al* [46]).

Pollak and Miller [75] and Pollak [76], while studying the average tunneling time in classical chemical systems, arrived to the concept of an imaginary time through the flux-flux correlation function. This imaginary time was equal to

$$\tau = -i\hbar\,{\rm Im}\frac{\partial \ln t}{\partial E}, \tag{101}$$

where t is the complex transmission amplitude.

We saw, with the help of the GF formalism, that the two characteristic times appearing in the Larmor clock approach correspond to the real and imaginary components of a single quantity, which we define as a complex traversal (or reflection) time. In the subsection on the oscillatory incident amplitude, we also discussed that Leavens and Aers [65] arrived to a complex barrier interaction time, Eq. (80), by studying the shape distortion of the transmitted wave by the barrier.

Nevertheless, it is in the Feynman path–integral approach where the concept of a complex time arises more naturally. Sokolovski and Baskin [66], using this kinematic approach to quantum mechanics, showed that a formal generalization of the classical time concept to the traversal time lead to a complex quantity.

The starting point for the Feynman path–integral approach [77] to the traversal time problem is the classical expression for the time that the particle spend in an arbitrary region $[0, L]$, which can be calculated through the expression

$$\tau_{0L}^{\rm cl} = \int_0^\tau \theta(y(t'))\theta(L - y(t'))dt', \tag{102}$$

where θ is here the step function, equal to 1 when its argument is positive and zero otherwise. The two θ functions ensure that we only count the time while the particle is in the barrier region. To use Eq. (102) in the quantum regime one has to generalize the expression for the classical time by replacing the classical trajectory $y(t)$ in the previous expression by a Feynman path and average Eq. (102) over all possible paths that start at position 0 on the left side of the barrier and end at position L at time t. Each path is weighted by the quantity $\exp\left(iS\{y\}\right)$, where

$$S\{y(t)\} = \int_0^t \left(\frac{m}{2}\left(\frac{dy}{dt'}\right)^2 - V(y(t'))\right)dt' \tag{103}$$

is the action associated with the path $y(t)$. As we are weighting each trajectory with a complex factor, it is natural to obtain a complex result for the average value. This weighting assumption has generated some controversies [4, 11, 78, 79]. Sokolovski and Baskin [66] arrived at the following complex time:

$$\tau_{0L} = i\hbar \int_0^L \frac{\delta \ln t}{\delta V(y)}\, dy, \tag{104}$$

where $\delta/\delta V(y)$ represents the functional derivative with respect to the barrier potential.

This result, Eq. (104), is strictly equivalent to expression (C16) for the integrated density of states, and so to our expression of the traversal time, as it is shown in Appendix C. Thus we can emphasize that this coincidence is quite natural, because in the tunneling time problem we always deal with an *open* and *finite* system. The functional derivative with respect to the potential appearing in Eq. (104) is equivalent to a derivative with respect to energy plus a correction term proportional to the reflection coefficient (see Eq. (47)).

The modulus of this expression, Eq. (104), is the time that Büttiker [45] obtained for the tunneling time in a square potential barrier and related to the Larmor clock times via:

$$\mathrm{Re}\, \tau_{0L} = \tau_y \tag{105}$$

$$-\,\mathrm{Im}\, \tau_{0L} = \tau_z. \tag{106}$$

Sokolovski and Connor [80] extended the Feynman path–integral approach to include the treatment of wavepackets. In their method the complex tunneling formally appears as a transition element $\tau_{0L} = \langle \Psi_\mathrm{F} | \tau^\mathrm{cl} | \Psi_\mathrm{I} \rangle$ between the initial wavepacket Ψ_I and the final one Ψ_F. Nevertheless, we have to note that Feynman and Hibbs [77] themselves do not associate any physical significance to transition elements.

Fertig [81, 82] avoided the problem of having to use wavepackets by considering restricted operators, for a fix energy or for a fix time. In this way, he was able to evaluate exactly the amplitude distribution for the traversal time for a rectangular barrier. He assumed that the weight of each path is proportional to $\exp\left(iS\{y\}\right)$, where the action S is given by Eq. (103). He obtained the following amplitude distribution for the traversal time [82]:

$$F(\tau) = \frac{1}{2\pi t(E, V_0)} \int_{-\infty}^{\infty} e^{-i\omega t} t(E, V_0 - \omega)\, d\omega \tag{107}$$

where $t(E, V_0)$ is the transmission amplitude at energy E through a barrier of height V_0. With this probability amplitude distribution for the average traversal time for the square potential barrier he arrives:

$$\langle \tau \rangle = -\frac{d\varphi}{dV_0} + \frac{i}{2} \frac{d \ln T}{dV_0}$$

which is the result of Sokolovski and Baskin [66].

The Wigner path distribution provides another approach to compute the traversal time. Jensen and Buot [83] used it to calculate the time for stationary waves, and Muga *et el.* [84] for wavepackets.

Bohm's interpretation of non-relativistic QM provides another kinematic path approach to evaluate the time. It is diametrically opposite to the fundamental concepts of "classical" QM according to the Kopenhagen interpretation which leads to Heisenber's uncertainty relation. In his interpretation an electron has a well defined position and velocity at each point in time, as in classical mechanics. But on the other hand, the electron's motion is described by a wave function, which satisfies the time-dependent Schrödinger equation containing the action S. Solving simultaneously the Schrödinger equation and the Hamilton-Jakobi equation one finds the motion of the classical particle in a modified potential, which is not the potential of the original problem. The modification of the potential and the fact that the classical paths in the Bohm approach do not cross are the starting points for the numerical simulation. The calculations have shown that the results of the Bohm trajectory approach and of the other approaches, e.g., the Larmor clock, are qualitatively different, even in the simplest case of a rectangular tunneling barrier. Generally Bohm's approach leads to larger traversal times than other approaches (see Leavens [6, 85]).

D Wavepacket Approach

The most direct method to calculate the delay time of a particle through a region is to follow the behavior of a wavepacket and determine the delay due to the structure of the region. This wavepacket approach has been criticized from different points of view, mainly due to the lack of causal relationship between the peaks or the centroids of the incident and transmitted wavepackets, and also because of the difficulties of an experimental set up to measure delay times. These critics are specially relevant for electronic waves. For example, the dispersive character of electron propagation has been claimed as responsible for the acceleration of wavepackets under appropriate circumstances. High–energy components of the packet travel faster and are transmitted more effectively than the other components, and so the transmitted packet comes almost entirely from the front of the incident packet. However, similar results were also obtained for dispersiveness electromagnetic waves (Ruiz *et al.* [15]). The fact that the transmitted wavepacket comes from the beginning of the incident wavepacket is mainly a consequence of interference effects.

At the same time, the results obtained from the wavepacket approach are similar to the results obtained with other more sophisticated approaches, and they present the advantage that can be easily generalized to

include finite size effects. In this section we review how to obtain delay times from the transmission coefficients.

Let us assume a region of interest, which in principle can be of any dimensionality, coupled to the outside by two 1D leads with a constant potential that we will assume equal to zero. We choose a coordinate system such that the incident lead extents from $-\infty$ to 0, and the other lead from L to $+\infty$.

A gaussian wavepacket of spatial width σ_1 is incident from the incoming lead on the region of interest. This packet is characterized by a wave function of the form:

$$\Psi(y,t) = \int_{-\infty}^{\infty} C \exp\left[-(k-k_0)^2/2(\Delta k)^2\right] \exp\left[iky - i\omega t\right]\, dk \tag{108}$$

where C is a normalization constant, k_0 the central wavenumber, $\omega = E/\hbar$, and $\Delta k = 1/\sqrt{2}\sigma_1$ is the spread of the packet in the wavenumber domain. The time evolution of this wavepacket is governed by Schrödinger equation. Nevertheless, the results are directly applicable to any other type of wave, including classical electromagnetic waves.

Part of the packet considered is transmitted and continues travelling outward along the second lead. Its wave function is given by:

$$\Psi(y,t) = \int_{-\infty}^{\infty} C|t(k)|e^{i\varphi(k)} \exp\left[-(k-k_0)^2/2(\Delta k)^2\right] \exp\left[iky - i\omega t\right]\, dk \tag{109}$$

$t(k)$ is the amplitude of transmission and $\varphi(k)$ its phase, which here we prefer to write as functions of the wavenumber k. The functions $t(k)$ and $\varphi(k)$ contain all the relevant information to calculate the delay time of the electronic wave function due to the region of interest.

While the general solution of the problem has to be obtained numerically, one can get close expressions for the time in the two extreme cases of very long and very short wavepackets, as compared with L. Very short packets travel as classical particles and their traversal times are given by the group velocity at the different regions considered, and taking into account possible multiple reflections. The delay time of very long wavepackets can be obtained from series expansions along the central wavenumber, what we will do next.

Let us assume that the wavepacket is so long that $t(k)$, $\varphi(k)$ and $\omega(k)$ only change smoothly on the scale of Δk. Then, in evaluating $|\Psi(y,t)|^2$, where $\Psi(y,t)$ is given by Eq. (109), we can expand $t(k)$, $\varphi(k)$ and $\omega(k)$ to second order in $k - k_0$.

We write the phase of the transmission amplitude as:

$$\varphi(k) = \varphi(k_0) + \tau_1(\omega - \omega_0) + \frac{1}{2}\tilde{\tau}_1(\omega-\omega_0)^2 \tag{110}$$

where ω_0 is the frequency corresponding to the central wavenumber k_0, τ_1 is the first derivative of the phase $\tau_1 = d\varphi(\omega)/d\omega$, and $\tilde{\tau}_1$ its second derivative $\tilde{\tau}_1 = d^2\varphi(\omega)/d\omega^2$.

Analogously, we write the modulus of the transmission amplitude as:

$$|\log t(k)| = |\log t(k_0)| + \tau_2(\omega-\omega_0) + \frac{1}{2}\tilde{\tau}_2(\omega-\omega_0)^2 \tag{111}$$

where $\tau_2 = d|\log t(\omega)|/d\omega$, and $\tilde{\tau}_2 = d^2|\log t(\omega)|/d\omega^2$. We can also expand the frequency ω in terms of k:

$$\omega = \omega_0 + v_{\rm g}(k-k_0) + \frac{1}{2}a_{\rm g}(k-k_0)^2 \tag{112}$$

$v_{\rm g}$ is the group velocity $v_{\rm g} = d\omega/dk$, and $a_{\rm g}$ its derivative with respect to k, $a_{\rm g} = d^2\omega/dk^2$. For electrons, the dispersion relation is given by:

$$\omega = \frac{\hbar k^2}{2m}, \tag{113}$$

so the group velocity is equal to $v_{\rm g} = \hbar k/m$, while the group acceleration is $a_{\rm g} = \hbar/m$. For photons, the group velocity is equal to the speed of light c and there is no acceleration, $a_{\rm g} = 0$.

If we keep terms up to second order in $k - k_0$ we can do analytically all the integrals appearing in the expression of the average value and the variance of y. After some trivial, but lengthy calculations we obtain that the average position $\langle y\rangle$ of the transmitted wavepackets as a function of time is given by:

$$\langle y\rangle = (t-\tau_1)v_{\rm g}\left[1 + \frac{\tau_2 a_{\rm g}}{b}\right] - \frac{\tau_2\tilde{\tau}_1 v_{\rm g}^3}{b} \tag{114}$$

where b is equal to:

$$b = \frac{1}{(\Delta k)^2} - \tau_2 a_{\rm g} - \tilde{\tau}_2 v_{\rm g}^2 \tag{115}$$

In the absence of dispersion, $a_{\rm g} = 0$, the traversal time is equal to τ_1, plus a small correction involving the second derivative of the transmission phase with respect to ω. This is in basic agreement with the expressions of the time obtained with other approaches, although we cannot obtain in this way the finite size correction proportional to the reflection amplitude. The dispersion introduces an acceleration since the factor multiplying the group velocity increases. This acceleration is proportional to the amount of dispersion, $a_{\rm g}$, and to the second component of the traversal time τ_2.

The variance of y of the wavepacket is equal to:

$$\sigma^2 = \frac{b}{2} + \frac{((\tau_1 - t)a_{\rm g} + \tilde{\tau}_1 v_{\rm g}^2)^2}{2b} \tag{116}$$

V. DWELL TIME

Until now we have concentrated on the traversal (transmission) and the reflection times, but there is also another important characteristic time called the dwell

time, about which there exists a vast literature (see, e.g., Landauer and Martin [11], Hauge an Støvnengd [4] and references therein). This time was first introduced by Büttiker [45], and is defined as the average number of particles within the barrier region divided by the average number entering (or leaving) the barrier per unit time. It corresponds to the average time spent by a particle within the barrier irrespectively of whether it is finally reflected or transmitted.

The dwell time in a neighborhood of y is defined as the ratio between the particle number in the interval $[y, y+dy]$ and the incoming current (Büttiker [45]):

$$d\tau^{(\mathrm{D})}(y) = \frac{|\psi(y)|^2}{J} dy \tag{117}$$

where $\psi(y)$ is the steady–state scattering solution of the time–independent Schrödinger equation, which outside the barrier has the form

$$\begin{aligned} \psi(y) &= e^{iky} + re^{-iky}, \;\; y < 0 \\ \psi(y) &= te^{iky}, \;\; y > L \end{aligned} \tag{118}$$

Obviously, Eq. (117) describes a balance equation: in the stationary case the injected current equals the decay rate of the probability in $[y, y+dy]$. The dwell time $\tau^{(\mathrm{D})}$ of a finite region within the context of a stationary–state scattering problem is obtained via a spatial integration of Eq. (117). So the dwell time $\tau^{(\mathrm{D})}$ is given by (Büttiker [45])

$$\tau^{(\mathrm{D})} \equiv \frac{m}{\hbar k} \int_0^L |\psi(y)|^2 \, dy, \tag{119}$$

Here the integral extends over the barrier, and $\hbar k/m$ is the incident flux.

Our aim is to calculate directly the dwell time, given by Eq. (119), for the case of a general one–dimensional asymmetric barrier for particles coming both from the left and from the right and to express the final result in terms of the scattering–matrix elements, given by Eq. (45).

Let us consider again a particle moving along the y–direction in the presence of an arbitrary potential barrier $V(y)$ in the interval $[0, L]$. In the interest of simplicity we do not consider the most general situation in which the potential energy for $y > L$ differs from zero and so we will assume that the potential is zero outside the barrier. We evaluate Eq. (119) in three steps, following the procedure of Ref. [86]. First, we incorporate the fact that the wave function appearing in this equation is a solution of Schrödinger equation. Second, we rewrite the wave functions in terms of Green functions. And finally, we express the Green functions in terms of the density of states and the reflection coefficients.

First of all, we take explicitly into account that the wave function appearing in Eq. (119) is a solution of the Schrödinger equation in the way we show in appendix C. Substituting Eq. (C10) for the integral over the barrier of the modulus square of the wave function in Eq. (119) we arrive at:

$$\begin{aligned} \tau^{(\mathrm{D})} = -\frac{\hbar}{4k} \Bigg[\psi^{*2}(y) \frac{\partial}{\partial E} \left(\frac{\psi'(y)\psi(y)}{|\psi(y)|^2} \right) \\ + \psi^2(y) \frac{\partial}{\partial E} \left(\frac{\psi^{*\prime}(y)\psi^*(y)}{|\psi(y)|^2} \right) \Bigg]_0^L . \end{aligned} \tag{120}$$

This expression is formally the same for particles incident from the left or from the right, but we have to remember that the corresponding wave functions will not be the same. García–Calderón and Rubio [87] arrived at the same result by a completely different method.

Our second step is to rewrite Eq. (120) in terms of the retarded GF $G(y, y')$ of the system, as we have been doing for the other times. Taking into account expressions (C7) for the GF in terms of wave functions and (C8) for the derivative of the GF we can write the first factor in the RHS of Eq. (120), containing the partial derivative with respect to the energy, as:

$$\begin{aligned} \frac{\partial}{\partial E} \left(\frac{\psi'(y)\psi(y)}{|\psi(y)|^2} \right) &= \frac{\partial}{\partial E} \left(\frac{\dot{G}(y+0, y)}{G(y, y)} \frac{\psi(y)}{\psi(y)^*} \right) \\ &= \frac{\partial}{\partial E} \left(\frac{-2m/\hbar^2 + G'(y, y)}{2G(y, y)} e^{2i\theta(y)} \right) \end{aligned} \tag{121}$$

where $\theta(y)$ is the phase function previously defined, Eq. (38), and which implicitly depends on energy. A similar expression is valid for the other factor in Eq. (120) containing the partial derivative with respect to the energy. Thus, using the previous expression and Eq.(C11) for the integral of the GF at coinciding coordinates, the dwell time can be written in terms of the GF as:

$$\tau^{(\mathrm{D})} = \left[i \frac{\partial}{\partial E} \theta(y) - G(y, y) \frac{\partial}{\partial E} \left(\frac{G'(y, y)}{G(y, y)} \right) \right]_0^L \tag{122}$$

As it occurs for the wavefunstion, the GF $G(y, y')$ depends on whether the particle arrives to the barrier from the left or from the right.

This technique was already applied to obtain the traversal time [57] and the dwell time [86] of an arbitrary barrier. After some cumbersome algebra, using Eqs. (C12–C15) and (C17), we arrive at the following result for the dwell time in terms of the transmission and reflection amplitudes:

$$\begin{aligned} \tau_-^{(\mathrm{D})} = \hbar \mathrm{Im} \Bigg\{ \left[\frac{\partial \ln t}{\partial E} + \frac{1}{4E}(r + r') \right] \\ + \frac{1}{2} \left[\sqrt{R} \frac{\partial}{\partial E} \ln \frac{r}{r'} + \frac{1}{2E}(r - r') \right] \Bigg\} \end{aligned} \tag{123}$$

The subindex $-$ indicates that the particle is coming from the left. r and r' are the reflection amplitudes from the left and from the right, respectively, R is the modulus square of these amplitudes $R = |r|^2 = |r'|^2$, and t is the transmission amplitude, which is independent of the incident direction as can be deduced from the time–reversal

and current conservation requirements [88]. When the particle is coming from the right, the dwell time is given by an expression similar to Eq. (123), but interchanging r and r'. We will refer to this case with the subindex $+$.

Gasparian *et al.* [57] showed that the first term on the RHS of equation (123) is proportional to the density of states. Then, we finally arrive at the following expression for the dwell time:

$$\tau_{\pm}^{(\mathrm{D})} = \pi\hbar L\nu(E) \pm \frac{\hbar}{2}\mathrm{Im}\left[\sqrt{R}\frac{\partial}{\partial E}\ln\frac{r}{r'} + \frac{1}{2E}(r-r')\right], \tag{124}$$

For a symmetric potential we have that the reflection coefficients from the right and from the left are equal, $r = r'$, and we obtain $\tau_{-}^{(\mathrm{D})} = \tau_{+}^{(\mathrm{D})} = \pi\hbar L\nu(E)$, in agreement with the result of Gasparian and Pollak [56].

For an asymmetric barrier, it is easy to check that the contribution from the asymmetry is the opposite for particles coming from the left and from the right. Then we find that:

$$\nu(E) = \frac{1}{2\pi\hbar L}\left(\tau_{-}^{(\mathrm{D})} + \tau_{+}^{(\mathrm{D})}\right) \tag{125}$$

This result was obtained in a much wider context by Iannaccone [89], which considered the relation between the dwell time and the density of states for a three–dimensional region Ω of arbitrary shape with an arbitrary number of incoming channels. He arrived at:

$$\nu_{\Omega}(E) = \frac{1}{2\pi\hbar}\sum_{n=1}^{N}\tau_{n}^{(\mathrm{D})} \tag{126}$$

where $\nu_{\Omega}(E)$ is the density of states per unit volume, and $\tau_{n}^{(\mathrm{D})}$ is the dwell time for particles coming from the n-channel. This result shows that the density of states in Ω is proportional to the sum of the dwell times in Ω for all the incoming channels.

A controversial question concerning the dwell time is to know whether it satisfies or not the relation (see Sokolovski and Baskin [66], Leavens and Aers [63] and Støvneng and Hauge [90]):

$$\tau^{(\mathrm{D})} = R\tau_{y,\mathrm{R}}^{\mathrm{BL}} + T\tau_{y}^{\mathrm{BL}}. \tag{127}$$

This result is trivial for classical particles, for which the traversal time coincides with the y component of our complex traversal time and for which there is no interference between the reflected and the transmitted particles. For the quantum coherent case, this result is not so clear. We can prove this relation, which we believe that it must hold because a particle incident on the barrier is either transmitted or reflected. Reflection and transmission of a particle are mutually exclusive events in the sense of Feynman and Hibbs [77]; that is, a measurement can determine, without interfering with the scattering event, whether a particle has been transmitted or reflected.

Our results for the y component of the transmission and reflection times, Eqs. (50) and (65), respectively, and for the dwell time, Eq. (123), allow us to prove exactly the previous relation between these times:

$$\tau_{-}^{(\mathrm{D})} = T\tau_{y}^{\mathrm{BL}} + R\tau_{y,\mathrm{R}}^{\mathrm{BL}} \equiv \mathrm{Im}\left\{\left[\frac{\partial\ln t}{\partial E} + \frac{1}{4E}(r+r')\right] + R\left[\frac{\partial}{\partial E}\ln\frac{r}{t} - \frac{1}{4Er}\left(1+rr'-t^2\right)\right]\right\} \tag{128}$$

On the other hand, our results also prove that the relation involving the full BL times

$$\tau^{(\mathrm{D})} = R\tau_{\mathrm{R}}^{\mathrm{BL}} + T\tau^{\mathrm{BL}}, \tag{129}$$

does not hold. This relation has been claimed very often in the literature, and also has been strongly criticized by other authors [11].

To close this section we briefly sketch a derivation of the initial expression of the dwell time, Eq. (119), deduced by Büttiker. We will follow the papers by Hauge, Falck, and Fjeldly [91] and by Leavens and Aers [92]. Let us assume once more a one–dimensional region of interest with a potential $V(y)$ in an interval $[0, L]$. The quantum mechanical probability for finding the particle on an arbitrary fixed interval $[0, L]$ at time t is (see, e.g., Landau and Lifshits [72])

$$P(0, L; t) = \int_{0}^{L}|\psi(y,t)|^2\,dy \tag{130}$$

Let us define the average time spent on $[0, L]$ by the particles described by the wavepacket $\psi(y, t)$ as

$$\langle\tau^{(\mathrm{D})}(0,L)\rangle = \int_{0}^{\infty}P(0,L;t)dt \equiv \int_{0}^{\infty}dt\int_{0}^{L}|\psi(y,t)|^2\,dy \tag{131}$$

We can expand the wavepacket $\psi(y, t)$ over the scattering states, given by Eq. (118), as:

$$\psi(y;t) = \int\frac{dk}{2\pi}\varphi(k)\psi(y;k)e^{-i\hbar k^2 t/2m} \tag{132}$$

where the coefficients $\varphi(k)$ determine the initial form of the wavepacket. Substituting this expression for the wavepacket in Eq. (131) we have [92]

$$\langle\tau^{(\mathrm{D})}(0,L)\rangle = \int_{-\infty}^{\infty}\frac{dk}{2\pi}|\varphi(k)|^2\frac{m}{\hbar k}\int_{0}^{L}|\psi(y)|^2\,dy \equiv \int_{-\infty}^{\infty}\frac{dk}{2\pi}|\varphi(k)|^2\,\tau^{(\mathrm{D})} \tag{133}$$

The last step proves that expression (119) for the dwell time is well justified.

We derived Eq. (133) from Eq. (131) assuming that the limits of integration over t extend from negative infinity to positive infinity. This makes no difference because when $\psi(0; t)$ is (essentially) zero for $y > 0$. The integration over t gives us a delta–function and the subsequent calculations can be performed readily. Thus $\langle\tau^{(\mathrm{D})}(0, L)\rangle$ is an average time spent in the barrier region, $0 \le y \le L$,

by a particle with wave function $\psi(y;t)$, with a probability $dk/2\pi\,|\varphi(k)|^2$ of having a wavevector between k and $k+dk$. Hence the Eq. (119) must be an exact expression for the average time spent in the barrier region by an incident particle of energy E regardless of whether it is ultimately transmitted or reflected.

VI. RECHARGING TIMES IN LOW DIMENSIONAL CLUSTER-ARRANGEMENTS

Apart from the fundamental questions involved in the QM concept of time and concepts of tunneling times, practical questions arise, with time related quantities as current in mesoscopic structures. Such phenomena can be observed in ME-devices working with SET. As already disclosed in 1.2, at present physical and chemical sub-10 nm nanostructures, e.g. ligand-stabilized clusters are favored for SET-devices. Before dealing with time in these ultimate structures, we have to recall some facts about usual single charge tunneling [31]: SE deals with small amounts of excess electrons on islands changing their distribution over the islands in time in a desirable way. In order to realize this the following two principal conditions must be fulfilled:

First, the insulating barriers separating conducting islands should be rather opaque. If the energy barrier is high enough (say, 1 eV) and $1-2$ nm in length, it provides essential decay of the electron wave function outside the island and, as a result, only weak overlapping of the wave functions of the neighbor islands occurs within the inter-island space. If besides this the number of electronic states contributing to tunneling is small enough then total exchange of electrons between the islands becomes negligibly small. This situation is often referred to the case of small quantum fluctuations of charge. In spite of relatively complex rigorous QM consideration, quantitatively this situation can be clearly formulated using such a characteristic of the tunneling junction as its tunneling resistance R_T. It should be much higher than the so called resistance quantum $R_q = \hbar/e^2 = 25.8\ k\Omega$. Then electrons in the island can be considered to be localized and classical electrodynamics can be applied, although their number is undergoing thermodynamic fluctuations as every statistical variable.

Second, in order to minimize these fluctuations and consequently to make the exchange of electrons controllable, the Coulomb energy associated with charging by one extra electron should be essential with respect to characteristic thermal energy kT. The Coulomb-, or electrostatic energy E_c of a charged conductor depends on its charge Q as well as on the size of the island and the capacitance of its nearest electrical environment. As long as the diameter of such an island is larger than the screening length of electrons, geometry dependence can be expressed solely by the resulting capacitance C of the insulated region. Then the Coulomb-energy of an extra charge $E_c = e^2/2C$ has to be $>> kT$. Thus usual lithographic SET-circuits with capacitances between $10^{-15}F - 10^{-16}F$ must be cooled down far below one Kelvin. SET at ambient temperature only can be achieved with capacitances between $10^{-18}F - 10^{-19}F$, typical for sub-10 nm microclusters (see 6.2).

If the above conditions are met, charge transport through this structure can be controlled by external voltage and current: Transfer of single electrons can be realized by means of QM tunneling if the probability of such tunneling depends on current biasing and driving voltages applied to the circuit.

A Transit time and recharging time in SET-junctions

In ME there is general agreement about the notion "transit time" which is independent of the mechanisms via which conduction takes place [19]. If we consider a region of a conductor in space with length $y_2 - y_1 = L$, between one point left and the other right, with electrons constantly being supplied from the left side and taken out on the right hand side, then, the magnitude of the total electron charge within this length is fixed by Q. Then current j_y can be defined by

$$j_y = \frac{dQ}{dt} \tag{134}$$

Herewith only the convenient assumption is made that each electrons spend the same amount of time $dt = \Delta\tau$ in travelling from left to right, where the time τ is called transit time.

In the present design of semiconductor devices and integrated circuits, transit times have been greatly reduced. Performance and limitations of operation speed as well as overall time constants of nanostructured switch elements are depending on transit times.

As for SET-devices, a single tunnel junction with length L and capacitance $C \approx L^{-1}$ and tunneling resistance R_T is the simplest system (fig. 6a). Then charging effects will appear if a current source supplies this junction with a charge independently of tunneling events by j_y.

Starting outside Coulomb blockade region, time dependant recharging of the junction occurs with

$$Q = \int j dt - Q_T$$

where the first term is the charge supplied by the source and the second term is the charge transferred through the barrier junction by tunneling which is regulated by the tunneling rate. In this place we recall the tunneling times which were discussed in chapters 1.3. and 2.2.1. Note, that in the present section we have already introduced transit time τ and furthermore we will discuss SET–period τ_{SET}, then recharging time τ_R, uncertainty

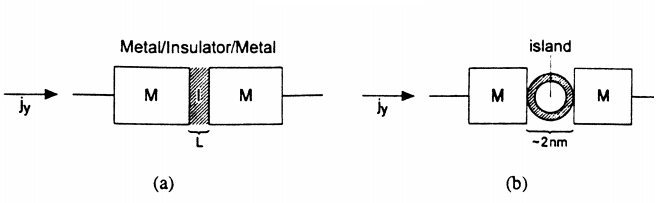

FIG. 6: a) Simplest system of a single metal/insulator/metal tunnel junction with length L. Charging effects will occur if a current source supplies this junction by j_y. b) Equivalent simplest tunnel–junction with a ligand stabilzed cluster (see fig.9) between the metal junction.

time τ_q and tunneling time τ_t, the latter are 3 types of times which are of different origin.

Since in metallic tunnel junctions tunneling timeτ_t with 10^{-15} sec is very short [55, 68], external recharging of the junction in time correlated SET will be periodic with the so called SET-tunneling frequency

$$\nu_{\rm SET} = \frac{j_y}{e} \tag{135}$$

Generally, the smaller the current, the more regular are the SET-oscillations, but with an inherent noise component due to the stochastic nature of the tunneling process.

Note, that transit time τ (134) refers to the "external" system around the single tunnel junction, supplying its current bias j_y. The tunnel junction system itself is characterized by "recharging time"

$$\tau_R = R_T C \tag{136}$$

Depending on the approach to recharging time, it may be defined either

- as a "decay time" of an excess charge which appears say on the right side of the barrier after a fast tunneling step (with finite but ultrashort traversal time in the order of 10^{-15} sec), forming a polaron-like state together with the "hole" it left on the left side, or
- as a "relaxation time" which the junction system needs to return to equilibrium, ready for a new cycle of external recharging. Thus recharging time and much faster tunneling time add in SET systems. Furthermore, transit time τ produced by the current bias system connected by j_y with relation (135) starting with $Q = 0$ at $t = 0$, adds to them also. Note, that $\tau_{\rm SET} = \nu_{\rm SET}^{-1}$ defines (in oscillating case) SET-period and thus a time depending on j_y (see fig. 7).

Typically, in nanostructured materials with the smallest possible conventional chip architecture ("classic" structuring techniques by shadow evaporation reveal a present day limit for SET-junctions of 30 nm x nm 30) the single tunnel junction comes up to a tunneling resistance $R_T \approx 10^5\ \Omega$ and with $L \approx 1-2\ nm$ a capacitance $C \geq 10^{-16}\ F$ is feasible. Thus recharging time with $\tau_R \approx 10^{-11}\ sec$ is still much larger than the tunneling time τ_t which an electron spends under barrier. An intermediate time scale is the "uncertainty time" $\tau_q = R_q C$, where R_q is the resistance quantum. The theory of SET assumes a clear separation of time scales $\tau_t \ll \tau_q \ll \tau_R$ (see fig. 8a). The first inequality states that the tunneling time is negligible and the second one states the classical nature of recharging by SET. According to Likharev [93], to maintain SET–oscillations meeting classical Eq. (135), SET–period with $\tau_{\rm SET} > 10\tau_R$ has to be at least ten times longer than recharging time. Otherwise amplitude and shape of the current oscillations will be more and more suppressed [93].

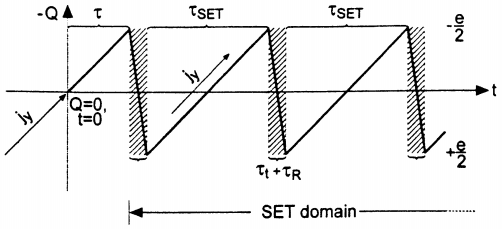

FIG. 7: External recharging of a tunneling junction by a current j_y. Oscillations are governed by the SET period $\tau_{\rm SET}$ and the system will be ready for a new cycle after a tunneling event with τ_t and recharging time τ_R. Transit time τ is only valid for the regime outside of SET domain.

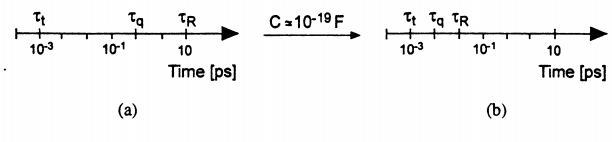

FIG. 8: a) The theory of SET assumes a clear separation of time scales $\tau_t \ll \tau_q \ll \tau_R$; b) For tunneling resistance R_T and small capacitances in the order of $10^{-19}F$ with ligand stabilized clusters, these three times may have the same order of magnitude.

B Time scale in ligand-stabilized cluster arrangements

With the availability of chemically size tailored quantum dots with a few nanometers in diameter, namely approximately spherical shaped ligand stabilized metal or semiconductor clusters in 3D- (solids or crystals), 2D- and 1D- (also in host- structures of nanoporous materials) or pair-arrangements and crystalline chalcogenide-clusters a new generation of nanoparticles and of ordered

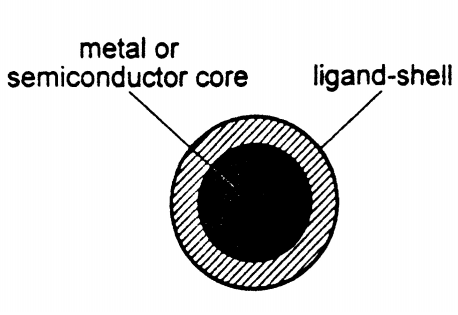

FIG. 9: Simplest model of a chemical nanostructure a ligand stabilized cluster.

materials was born. One typical, well investigated representative is Au_{55} with a core diameter of 1.4 nm and a double ligand shell-thickness of 0.7 nm (see fig. 9), the latter adjustable to more by more volumes ligands or by chemical spacers. Impedance Spectroscopy (IS) experiments and tunneling of single clusters revealed SET at room temperature confirming the theoretically expected inter-particle capacitance C (respective the self capacitance C_0 to ground), in the order of magnitude of 10^{-18} F down to 10^{-19} F. By IS–experiments this value can be evaluated both from activation enthalpy or from the density of states contributing to the process. Strictly speaking, this capacitance is not homogeneous and not classically defined. Nevertheless the (shell-) capacitance and with it the Coulomb-barrier $e^2/2C$ can be controlled by thickness of the ligand-shell and by the diameter d of the metallic (or semiconductor) core. The core in general is characterized by metallic behavior (the species with larger numbers of metal atoms > 100) or semiconducting behavior (small metal clusters and metal-chalcogenides). The smallest microclusters with a core diameter $d < 1$ nm are quantum dots where electrons with standing waves (ground state $\lambda/2 = d$) are confined with discrete energy levels. Since the number of atoms is restricted to less than 100 and moreover since most of them are surface atoms bound to the ligand shell, anyway one only can expect < 100 conductance electrons per cluster.

In first approximation the capacitance $C_{\rm micro}$ of interacting ligand-stabilized quantum dots in solids obeys Kirchhoff's laws [33]. Cubes of ordered densest 3D-arrangements of ligand- stabilized clusters or crystalline materials show an overall capacitance of approximately $nC_{\rm micro}$ (n the equal number of clusters in each space direction). Various other arrangements with inter–particle capacitance for SET, e.g. parallel chains with self capacitances C_0 (again in the same order of magnitude as $C_{\rm micro}$) in between, and tunnel barriers with inter-particle capacitances $C_{\rm micro}$ along the arrays are discussed [94].

More complicated is the estimation or the measurement of the particle resistance R_p (to junctions, to ground or between building units of a cluster arrangement) which may have very small values in the order of magnitude of quantum resistance R_q up to typical tunneling resistances R_T in the range of $M\Omega$. In the case of low resistance, conductance may reveal band structure for single electrons (similar to minibands) [33].

Note, that with clusters being nanoparticles, the above two principal conditions for "classical" SET need modification (see Simon and Schön [18]):

- First, such a simple parameter as a constant tunneling resistance R_T must be handled with care.

- Second, the Coulomb energy only roughly can be described by the elementary formula for the charging energy of a capacitor. Then the symbol C denotes an amount which generally depends on the number of interacting electrons occupying the cluster.

However, these peculiarities of metal nanoparticles do not eliminate charging effects. The SET-effect and the quantum size effect do not contradict each other, and can coexist. The effect of discrete levels on the charging characteristics has been treated by Averin and Korotkov [95], who extended the theory of correlated SET to small nanoparticles. But as we will discuss in the following sections, description of the effect with an adequate time-scale will be much complicated when characteristic recharging times R_T C become as short as the characteristic time of the energy relaxation inside the quantum dot.

1 SET-junction with a single cluster

Let us first discuss the situation of one single ligand stabilized cluster in between the metal junctions (see fig. 6b). The figure suggests a symmetric two tunnel junction system with at least two capacitances and one island. But one must remember that actually the ligand-shell capacitance $C_{\rm micro}$ is approximately spheric. Anyhow, in electrical engineering terms by circuit equivalent approach it should behave like the simplest case of one single junction (see fig. 6a) with capacitances coupled to C which is close to $C_{\rm micro}$.

Let us again discuss the three relevant times:

- The tunneling time τ_t, as above mentioned, will be $\tau_t \approx 10^{-15} sec$.

- The recharging time $\tau_R = R_T C = R_T C_{\rm micro}$. This again may be the longest time (see fig.8a). But in special cases (e.g. for clusters with $C_{\rm micro} = 10^{-19} F$ and very low $R_T \leq 10^5$ Ω), we get

$$\tau_R \leq 10^{-14}\ sec \tag{137}$$

Note, that the capacitance contribution to τ_R depends on chemically tailoring and spacing to next cluster neighbors (as well as the resistance involved) and on the nature of the ligand-shell, e.g. its thickness or charge. This was proved by experiments with Au_{55} and Pt_{561} with chemically different ligand shells and different spacers [96].

- Furthermore we must consider the before mentioned "uncertainty time" $\tau_q = R_q C_{\rm micro} = \hbar C_{\rm micro}/e^2$ associated with the Coulomb energy, a quantity for the electron

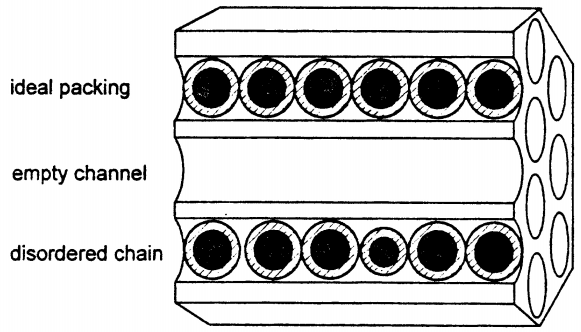

FIG. 10: Arrays of ligand stabilized clusters as guest arrays in a nanoporous solid: ideal packing and disordered chain with local defects in distance and cluster size.

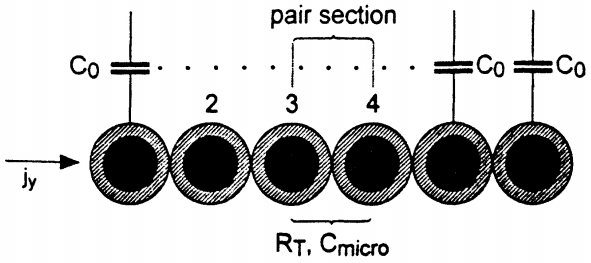

FIG. 11: 1D–array of ligand stabilized Au_{55} clusters with inter–particle capacitance $C_{\rm micro}$ and self capacitance C_0 (to neighbors or to ground). A pair section e.g. between clusters 3 and 4 can be regarded as one SET–junction.

fluctuations of any electrons involved in the recharging and tunneling mechanism

$$\tau_q \approx 10^{-14} sec \tag{138}$$

Now, with approximately 10^{-14} *sec*–10^{-15} *sec* all three times are in the same order of magnitude with $\tau_t \approx \tau_q \approx \tau_R$ (see fig.8b). For microcluster SET-junctions we do no longer know which time scale is relevant. This is not only of theoretical interest but also very important for practical application in cluster-ME. Since, within a cluster arrangement we should know wether, and in which time a single-electron signal starting at $t = 0$, arrives to a receiver, if this receiver is one next neighboring cluster-unit. In that case, we disregard transit time of the environment of such an arrangement.

2 1D-cluster arrays

Let us focus our interest to an artificial arrangement of an isolated 1D-cluster chain with a number of n clusters. Such a multiple tunnel junction arrangement is within experimental reach as there were grown chains of clusters [97] and since such chains may exist in anisotropic cluster crystals (with spacers) or as guest arrays in nanoporous inorganic host-structures (see fig.10) [3]. Even in compressed discs of ligand stabilized Au_{55} clusters there are regions of high order with densest package [33] and SET-features (including fine structures due to energy quantization) were visible [98]. In monolayers of Au_{55} clusters also were observed a short range close packing with a correlation length of the cluster arrays up to 40 nm ($n = 20$) [99] and SET- phenomena [100]. Regarding a single electron entering this chain, we are interested in the time or velocity relevant for the propagation of the electron which passes the array in a soliton-like state:

Let us first look at an 1D-array of ligand-stabilized Au_{55} clusters (see fig.11) with small inter-particle capacitance $C_{\rm micro}$ say as a current path through a 3D-arrangement (self-capacitance $C_0 \approx C_{\rm micro}$). Any single section of a pair of clusters of this periodic chain structure in the direction of current j_y can be regarded as one single SET-junction separated by their own (double) ligand shells.

3 High inter-particle resistance R_T in condensed cluster phase

IS-measurements at different species of condensed Au_{55} proved a circuit equivalent for the total capacitance of the samples obeying Kirchhoff's laws [33, 97]. Thus local microscopic capacitance $C_{\rm micro}$ could be destined in accordance to later STM-measurements on single Au_{55} clusters [100]. On the other hand, direct evaluation of local inter-particle resistance R_T was not possible since sample resistance revealed no clear dependance from volume. Instead, macroscopic relaxation frequencies in the 100 kHz-region changed with thickness of the sample or respectively with the distance of electrodes, leading to a picture of percolating current paths or channels oriented to the electric field [33, 101, 102]. All these experiments are suffering under disorder and imperfect arrangement of clusters and, therefore, relatively broad distributions of macroscopic relaxation times $\tau_{\rm macro}$ are appearing. Measurements at air–sensitive and metastable single-crystals of metal chalcogenide clusters do not permit a clear decision between intrinsic electronic processes or conductivity caused by impurities [96].

Nevertheless, at present, the picture of (parallel) current channels in quasi 1D-cluster arrays between the electrodes seems to be most suitable to experiments since $\tau_{\rm macro}$ then can be simply explained as an operation time needed for the (single) electron transport from one electrode to the other. Thus, we have

$$\tau_{\rm macro} \approx n\tau_R = nR_T C_{\rm micro} \tag{139}$$

¿From one typical measurement [32] at Au_{55} ($\tau_{\rm macro} \approx 10^{-5}$ *sec*, $n \approx 10^5$ and $C_{\rm micro} \approx 10^{-18} F$), we obtain

$R_T \approx 100\ M\Omega$, in good agreement with Ref.[100]. Experiments or rather Eq.(139) express that with high inter-particle resistance R_R in densest cluster-arrangements, recharging time τ_R rules over SET-time $\tau_{\rm SET}$, thus we can explain it as the relaxation time which the cluster-pair junction needs to return to equilibrium (see 6.1.). Thus operation time for one cluster-pair section with high tunneling resistance R_T will be given by recharging time τ_R.

Minimal recharging time τ_R and maximal operation speed will be hypothetically approached with $R_T \to R_q$. Let us estimate maximum electron "velocity" as a clue in classical terms between neighboring clusters with $\tau_R \approx \tau_t$ (see 6.2.1): $v_e \approx L/\tau_R$.

Tunneling barrier L, $\lambda/2$, $2R$ (and so on) are in the order of 1 nm. Hence $v_e \approx 10^6 m/s = 10^{-2}c$. It is interesting to note that in this case we expect the same electron velocity v_e as in the ballistic transport case in semiconductors [103]. Moreover, we find a situation similar to Bohr's original semi-classic atom model for the electrons on circular orbits, with 1% of light velocity c. This means that we do not need to take into consideration relativistic effects.

Let us consider now, as a whole, the before 1D-cluster array, with small inter-particle capacitance $C_{\rm micro}$ as an isolated chain (self capacitance $C_0 \approx 0$).

4 Isolated chains with low inter-particle resistance R_T or R_q

First, if the inter-particle resistance R_T is still high enough to meet condition $\tau_{\rm SET} > 10\tau_R$, the situation of a very high frequency SET-turnstile device is given, where Coulomb barrier has to be overcome only once.

Secondly, interesting questions arise with the case $R_T \to R_q$, since quantum wires surely can be chemically tailored by suitable ligand-shells and spacers (see 6.2.1). Now the time-dependent play between slowly refilling a reservoir (a SET- island), fast tunneling and recharging of the junction is definitively over since one of the prerequisites of SET is no more satisfied. Then the electron tends to go into a delocalized state and τ_R is no longer a relevant quantity.

To handle this problem we start with the question: Which collective total resistance can be attributed to the above chain? To answer this question we have to visualize that even in arrays, which are fabricated by lithographic techniques in the sub-micron range, the device dimensions are smaller than the inelastic scattering length of the conductor materials of which they are composed. Thus, charge transport is governed by coherent wave propagation, whereby elastic scattering leads to - macroscopic observable - quantum interference effects. With respect to an 1D-array, the resistance will fluctuate with portions in the order of quantum resistance R_q, depending on the position and distribution of elastic scattering centers. In an array of ligand-stabilized clusters

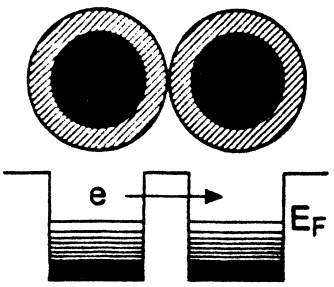

FIG. 12: Two neigboring clusters idealized as two quantum wells with a tunneling barrier in between. Single electrons near Fermi level E_F may tunnel depending on biasing.

these may be e.g. packing defects, i.e. fluctuations in capacitance $C_{\rm micro}$ [94].

Some scientists believe that the length-independent resistance quantum $R_q = \hbar/e^2$ is connected with the electron motion in the ground state of the most elementary anharmonic electron resonator: the s-orbital of the hydrogen atom [104]. Similar to Bohr's model of the hydrogen atom with the first K-shell, we can speak of s-electrons in "cluster"–σ–orbitals [33]. This concept means that wave functions exist, which are in turn tailored by the size and shape of the cluster [105, 106]. Consequently, to such an elementary harmonic electron resonator, the resistance quantum R_q may be attributed also [33] as well as to the propagation of single electrons in an ideal array with inter-particle resistance R_q. On the other hand it has been shown [60] that the resistance R_a of an 1D-array in the case of a defined potential difference on its edges is expressed by

$$R_a = \frac{\hbar}{2e^2 T} \tag{140}$$

where T is the energy averaged transmission probability. This also implies, in the absence of disorder that the total resistance of a size tailored periodic 1D cluster array at low temperature may be $\hbar/2e^2$. A combination of low resistance and low temperature variation of the resistance is expected to be of enormous importance in ME-device design [107].

If we regard again the concept of recharging time after tunneling, we have to realize that it is now failing in its strict sense: The former recharging times τ_R of single cluster sections of the array are now converted into uncertainty time τ_q, if we disregard from recharging time of the electrodes which serve as reservoirs supplying and equilibrating the charges resulting from the potential difference applied to the array. Although, however, in real systems the macroscopic recharging time may still roughly be expressed by $nR_qC_{\rm micro}$.

5 *Measuring of ultrashort recharging times*

With regard to Eq.(139), one might have the idea to measure ultrashort recharging times by macroscopic relaxation time, similar to the IS-measurements described in section A with high inter-particle resistance R_T. With $R_T \to R_q$ relaxation frequencies would be expected in the 1 GHz-region. Experiments could be done at an adequate array (or a bundle of chains) of Q–dots of ligand-stabilized clusters (say arranged in a crystal or in channels of a host structure), by dividing macroscopic relaxation time by the number of chain members n. But we must be aware that then, because of $\tau_t \approx \tau_R \approx \tau_q$ we always measure a sum of times, but it would be an access to the order of tunneling time. Since until now, there exist no tunneling time experiments at such arrays, the above suggestions may lead to qualitative approximation.

We emphasize that the above simple considerations only make sense for approaching (to make transparent) this new field of chemical quantum dot arrangements figuratively speaking. Of course they are not adequate to replace still missing analytical calculations of fast tunneling problems with possible "superluminal" speed in periodic chemical nanostructures, we indicated in 1.5.

6 *The cluster-pair switch*

The simplest and smallest but hypothetical one-dimensional SET- device with an area of 2 nm x 4 nm which was discussed recently [33] is the two-cluster switch, consisting of a pair of small ligand-stabilized metal clusters separated by their own ligand-shells. It corresponds e.g. to one pair section of fig.11, say clusters 3 and 4. Its principle is sketched in fig.12. The probability of tunneling of one electron out of the left side quantum well into the right side well depends on biasing and on distribution of excess electrons over sites. Again, with microclusters there are only few "conducting" electrons available at Fermi level E_F in both reservoirs. For current switching, one excess electron must pass the tunnel–barrier. With respect to 4.2. it is interesting to see that discrete energy modulation of the barrier can be used to create a discrete spectrum of particle energies in the next quantum–well.

VII. NUMERICAL RESULTS

We have divided this section into two parts. The first one corresponds to the long wavepacket limit, when the spread of the wave function is longer than the size of the system and then expressions (47) and (67) for the traversal and reflection times respectively are valid. In this case, the numerical problem reduces to the evaluation of the transmission and reflection amplitudes and their energy derivatives, which can be conveniently achieved through the use of the characteristic determinant method, introduced by Aronov and Gasparian [58] and explained in appendix A. Different similar mathematical methods, allowing us to take into account multiple interfaces consistently and exactly without the use of perturbation theory, have been proposed. For example, Garcia-Moliner and Rubio [108] and Velicky and Bartos [109] introduced a method, based on the surface Green functions, to study the energy spectra of electrons in systems containing interfaces between different crystals. This method has been applied to various problems in solid state physics before [110, 111, 112, 113].

The second part of this section concentrates on finite size effects and in this case we have to consider a specific wavepacket and evaluate its probability amplitude at different values of the time in order to calculate the amount of time taken to cross the system.

A Long wavepackets

The evaluation of equations (47) and (67) for the traversal and reflection times can be performed directly for simple systems or with the help of the characteristic determinant for more complex systems. Here we review the results for a rectangular barrier, for a finite periodic system and for two barriers, i.e., for resonant tunneling.

1 *Results for a rectangular barrier*

In the section on the Larmor clock, we gave the explicit expressions for the y and z components of the traversal time corresponding to a rectangular potential barrier, Eqs. (22) and (21). In Fig. 4 we showed the variation of these times as a function of energy. These expressions refer to under barrier transmission. For energies above the potential of the barrier, the analytical continuation of these expressions apply. In this case, the traversal times oscillate with energy. We can calculate the average of τ_1 exactly and check that it is equal to the classical crossing time without including reflections, i.e., to the time taken by the first pulse to cross the barrier in the limit of very short pulses.

2 *Periodic structure*

We now consider a periodic arrangement of layers. Layers with potential V_1 and thickness d_1 alternate with layers with potential V_2 and thickness d_2. We assume that the energy is higher than $\max\{V_1, V_2\}$, and so the wavenumber in the layers of the first and second type is $k_i = [2m(E - V_i)]^{1/2}/\hbar$ $(i = 1, 2)$. In this case, the results for long wavepackets apply equally well to electromagnetic waves considering $k_i = \omega n_i/c$, where n_i is the indice of refraction of the two types of layers. Let us

call a to the spatial period, so $a = d_1 + d_2$. The periodicity of the system allows us to obtain analytically the transmission amplitude using the characteristic determinant method [49]:

$$t = e^{-ik_1 d_1} \left\{ \cos(N\beta a/2) - i \frac{\sin(N\beta a/2)}{\sin \beta a} \times \sqrt{\sin^2 \beta a + \left[\frac{k_1^2 - k_2^2}{2k_1 k_2} \sin k_2 d_2 \right]^2} \right\}^{-1} , \quad (141)$$

where β plays the role of quasimomentum of the system, and is defined by

$$\cos \beta a = \cos k_1 d_1 \cos k_2 d_2 - \frac{k_1^2 + k_2^2}{2k_1 k_2} \sin k_1 d_1 \sin k_2 d_2 \, . \quad (142)$$

When the modulus of the RHS of Eq. (142) is greater than 1, β has to be taken as imaginary. This situation corresponds to a forbidden energy band. The term within brackets in Eq.(141) only depends on the properties of one barrier, while the quotient of the sine functions contains the information about the interference between different barriers. The transmission coefficient is equal to 1 when $\sin(N\beta a/2) = 0$ and β is different from 0. This condition occurs for

$$\beta a = \frac{2\pi n}{N} \qquad (n = 1, \cdots, N/2 - 1) \, , \quad (143)$$

and we say that it corresponds to a resonant frequency.

For the reflection amplitude we have

$$r = te^{-ik_1 d_1} \frac{k_1^2 - k_2^2}{2k_1 k_2} \sin k_2 d_2 \frac{\sin(N\beta a/2)}{\sin \beta a} \, . \quad (144)$$

With these expressions for the transmission amplitude, Eq. (141), and for the reflection amplitude, Eq. (144), we can calculate the traversal time through equation (47) and the reflection time via equation (67).

We concentrate in the simplest periodic case, which corresponds to the choice $k_1 d_1 = k_2 d_2$. This case contains most of the physics of the problem and is also used in most experimental setups [9]. From Eqs. (141) and (144), Ruiz *et al.* [15] calculated numerically the traversal time for electromagnetic waves considering a system of 19 layers ($N = 20$) with alternating indices of refraction of 2 and 1, and widths of 0.6 and 1.2, respectively. Their main conclusions are also applicable to the problem of an electron in a periodic potential. In Fig. 13 we represent τ_1 and τ_2 for electromagnetic waves in a periodic system as a function of k_1. In the energy gaps, the traversal times are significantly smaller than the crossing time at the vacuum speed of light (horizontal line). The average of τ_1 with respect to wavenumber is equal to 22.8, and coincides with the classical crossing time, i.e., for very short wavepackets, without including multiple reflections. It corresponds to the horizontal straight line in Fig. 13.

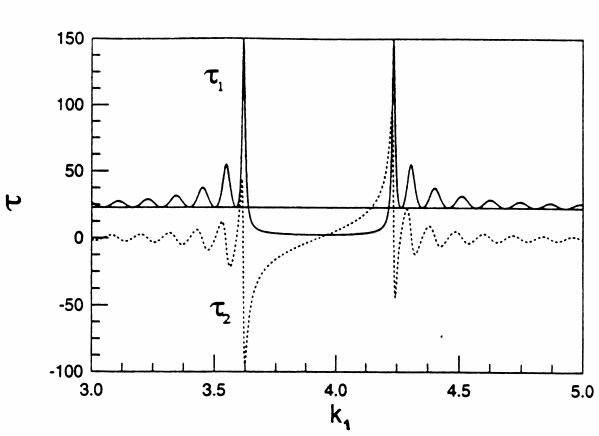

FIG. 13: Traversal times versus the size of the wavepacket for a periodic system. The solid line corresponds to τ_1, and the dashed line to τ_2. The values of the parameters are $N = 20$, $n_1 = 2$, $n_2 = 1$, $d_1 = 0.6$ and $d_2 = 1.2$.

3 *Resonant tunneling*

Double–barrier potential structures present resonant tunneling, which has been studied for electrons since the early days of quantum mechanics [90, 114, 115]. Resonant tunneling for electromagnetic waves is easier to carry out than corresponding experiments on electrons [26].

A double–barrier structure is a special case of a periodic system consisting of $N = 4$ interfaces with two evanescent regions separated by a propagating one. In the evanescent layers the potential energy V_2 is larger than the energy of the electron E. The results of the previous part also applied to this case where one type of layers are evanescent. We merely have to replace k_2 by $-i\kappa$ where $\kappa = [2m(V_2 - E)]^{1/2}/\hbar$(correspondingly, $\sin k_2 d_2$ becomes $\sinh \kappa d_2$.)

Cuevas *et al.* [49] calculated the traversal time τ for electromagnetic waves through a double barrier structure using the previous equations for the transmission and reflection amplitudes, Eqs. (141) and (144) with $N = 4$, convoluted with a gaussian distribution function with a standard deviation of 6 MHZ, which reproduces the same average height of the peak as the corresponding experiments [26].

The behavior of the traversal time at a resonance is fairly universal. The phase of the transmission amplitude changes by an angle of π at each resonance, as predicted by Friedel's sum rule. Its frequency dependence can be fitted quite accurately by an arc tangent function. The time, proportional to the derivative of this phase, is a Lorentzian with the same central frequency and width as the Lorentzian corresponding to the transmission coefficient. As the lifetime τ_l of the resonant state is the inverse of the width of the transmission coefficient at half

maximum, we conclude that it must be equal to half the traversal time at the maximum of the resonant peak

$$\tau_1 = \frac{1}{2}\tau_{\rm res} \ . \tag{145}$$

This result was obtained by Gasparian and Pollak [56] by considering the traversal time for an electron tunneling through a barrier with looses, i.e., with a decay time.

B Finite size effects

The kinetic approach is suitable to study numerically the evolution of wavepackets with sizes of the order of the width of the region of interest. Up to now this has only been done neglecting dispersion [15]. This is not very adequate for electrons, although the results show some light on very interesting aspect of the problem, so we include them here.

We will describe the numerical simulations of the time evolution of finite size wavepackets that cross the region of interest and measure the delay of the peak of the transmitted wave as a function of the size of the original packet. The simulations also calculate the change in size of the packets. As we are not including dispersion effects the results are directly applicable to electromagnetic waves, so we will use a nomenclature most appropriate for them, although the results are equally valid for electrons, in the absence of dispersion, provided that we translate indices of refraction into their corresponding potentials.

Let us consider a three-dimensional layered system with translational symmetry in the $Y-Z$ plane, and consistent of N layers labelled $i = 1, \ldots, N$ between two equal semi–infinite media with a uniform dielectric constant n_0. The boundaries of the i–th layer are given by y_i and y_{i+1}, with $y_1 = 0$ and $y_{N+1} = L$, so that the region of interest corresponds to the interval $0 \le y \le L$. Each layer is characterized by an index of refraction n_i. In the case of electrons, we assume that the energy E of the electron is higher than the potentials of the different layers and that the wavenumbers are inversely proportional to the indices of refraction; so the potential V_i in layer y is equal to $V_i = E(1-(n_0/n_i)^2)$.

One calculates the position of the packet at different times and from this information one extracts the time taken by the packet to cross the region of interest. In particular, neglecting dispersion, one can measure the average positions $\overline{y}_1$ and $\overline{y}_2$ of the square of the modulus of the wavepacket at two values of t, t_1 and t_2, such that the packet is very far to the right of the structure at t_1 and very far to the left at t_2. These average positions are defined as

$$\overline{y}(t) = \int_{-\infty}^{\infty} y|\Psi(y,t)|^2\, dy \tag{146}$$

The traversal time of the wavepacket through the region of interest is given by:

$$\tau = t_2 - t_1 - \frac{(\overline{y}_2 - \overline{y}_1 - L)n_0}{c}. \tag{147}$$

Although we refer to this time as a traversal time, it is learn that, strictly speaking, is a delay time. Part of the interest of this type of simulations is to study how delay times relate to the previously obtained expressions for the traversal time.

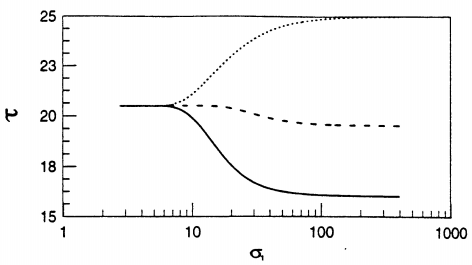

FIG. 14: Traversal time versus the size of the wavepacket for a rectangular barrier. The dashed line corresponds to a central wavenumber $k = 81\pi/80$, the solidd line to $41\pi/40$, and the dotted line to $21\pi/20$. The values of the parameters are $L = 10$, $n = 2$ and $n_0 = 1$.

1 *Rectangular barrier*

Let us consider first finite size effects for a rectangular barrier or slab confined to the segment $0 \le y \le L$ and characterized by an index of refraction n.

In Fig. 14 we plot the traversal time versus the size of the wavepacket for three different values of the central wavenumber, $k = 81\pi/80$ (dashed line), $41\pi/40$ (solid line) and $21\pi/20$ (dotted line). The values of the parameters are $L = 10$, $n = 2$ and $n_0 = 1$, and the velocity is supposed equal to 1. The values of the wavenumbers are chosen so that $\sin 2u = 1$, $\sin u = 1$ and $\sin u = 0$, and so the characteristic time τ_1 is a central value, a minimum and a maximum, respectively. We can check that the long wavepacket limit of these results corresponds to the value of τ_1, given by Eq. (21).

The traversal times of very short pulses are all equal to 20.8, independently of the central wavenumber considered. This value is the classical crossing time, taking into account multiple reflection, which for the slab is given by:

$$\tau = \frac{Ln}{c}\frac{1+|r|^4}{1-|r|^4} \ . \tag{148}$$

The transition between the long and short wavepackets limits takes place for wavepacket's sizes of the order of 20, i.e., of the order of the width of the slab.

The transmission coefficient presents a similar behavior to the traversal time [15]. In the regions with destructive interference, so that the transmission coefficient is very small, the crossing times are also very small.

2 Periodic structure

We now consider finite size effects in the periodic arrangement of layers previously study in the subsection on Long wavepackets. Layers with index of refraction $n_1 = 1$ and thickness d_1 alternate with layers of index of refraction $n_2 = 2$ and thickness d_2.

In Fig. 15 we show the delay time versus the size of the wavepacket for two values of the central wavenumber, $k_0 = 3.927$ and $k_0 = 4.306$, which correspond to the center of the gap and to a resonance, respectively. There is again a strong similarity in the behavior of the traversal time and of the transmission coefficient [15]. The long wavepacket limit of the traversal time coincides with the characteristic time τ_1, while the short wavepacket limit is independent of wavenumber and equal to 29.

The speed of the wave is greater than in vacuum for a wide range of sizes. The minimum size of the packets that travel faster than in vacuum is about 9, so that the corresponding width $2\sigma_{\rm I}$ is very much the same as the size of the system. Velocities larger than in vacuum occur when the transmission coefficient is very small. In regions with a very small density of states the traversal time is very short and, at the same time, transmission is very difficult due to the lack of states at the corresponding energies.

The width of the transmitted packet $\sigma_{\rm T}$ is slightly smaller than the width of the incident packet $\sigma_{\rm I}$. According to the results in the subsection on the wavepackt approach, we obtain that, in the absence of dispersion and up to second order in perturbation theory, this change in width depends on the derivatives with respect to frequency of τ_1 and τ_2. As the first of these derivatives is equal to zero in the centre of the gap, one arrives at:

$$\sigma_{\rm T}^2 = \sigma_{\rm I}^2 - \frac{v_{\rm g}^2}{2}\,\frac{d\tau_2}{d\omega}\,. \qquad (149)$$

In order to check up to which sizes second order perturbation theory is valid, Ruiz *et al.* [15] plotted $\sigma_{\rm I}^2 - \sigma_{\rm T}^2$ as a function of the size of the packet and compared it with the value of $(1/2)(d\tau_2/d\omega)$ obtained from the characteristic determinant. Second order perturbation theory works adequately for a wide range of sizes and, in particular, for the sizes for which one obtains velocities larger than in vacuum.

The error in the measurement of the traversal time of a single wavepacket is its width divided by its velocity. All the packets that travel faster than in vacuum are so wide that their uncertainty in the traversal time is larger than the traversal time itself and even larger than the time it would take a wave to cross the structure travelling at the same speed as in the vacuum.

VIII. CONCLUSIONS AND OUTLOOK

In this review we have discussed the topic of tunneling time in mesoscopic systems including nanostructures,

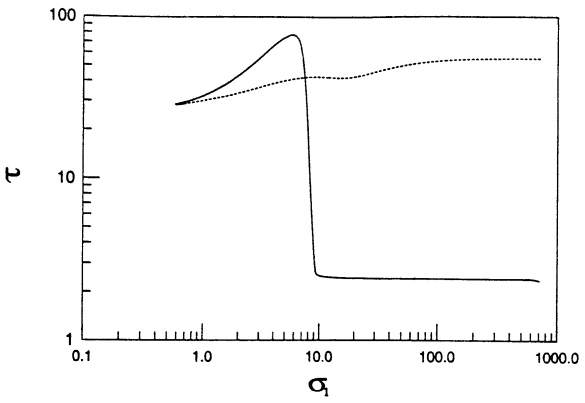

FIG. 15: Traversal time versus the size of the wavepacket for a periodic system. The solid line corresponds to a central wavenumber $k = 3.927$, and the dashed line to $k = 4.3$. The values of the parameters are the same as in figure 12.

particularly in 1D systems with arbitrary shaped potential. But the treatment of tunneling time in "nanostructured materials" approaching the molecular and atomic scales is still open.

In the field of tunneling time there are problems in any of the existing approaches, and we do not have a clear answer for the general question "How much time does tunneling take?". Unfortunately no one of these approaches is completely adequate for the definition of the time in QM. Nevertheless, we note that all these different approaches can be consistently formulated in terms of Green's function, and their main differences can be fairly well understood.

As we have pointed out in sections 1.2 and 6 great progress in the application of ligand stabilized microcluster quantum dots in SE was reached recently. Therefore it seems that the race between "physical" and "chemical" nanostructured materials was decided in favor of chemistry: At present, the physical requirements for further investigation of nanostructured tunneling devices can be satisfied by chemically size tailoring zero-, one-, two- or higher dimensional cluster materials in mole scale, although fabrication techniques for hybrid or pure cluster-nanodevices are still lacking.

A Complex nature of time

For 1D systems we obtained closed expressions for the traversal and reflection times, Eqs. (47) and (67), in terms of partial derivatives of the transmission and reflection amplitudes with respect to energy. Results of other approaches can be related to these expressions and the main differences can be grouped into two categories: the complex nature of time and finite size effects.

Our conclusion about the complex nature of time is the following. It is clear that there are two characteristic times to describe the tunneling of particles through barriers. (Similar conclusions can be reached for reflecting particles.) These two times correspond to the real and imaginary components of an entity, which we can choose as the central object of the theory. Different experiments or simulations will correspond to one of their components or to a mixture of both. Büttiker and Landauer argue that these two times always enter into any physically meaningful experiment through the square root of the sum of their squares, and so claim that the relevant quantity is the modulus of the complex time.

B Finite size effects in mesoscopic systems

As regards to finite size effects, we believe that Eqs. (47) and (67) are exact, and adequately incorporate finite size effects. These effects correspond to the terms which are not proportional to derivatives with respect to energy. They are important at low energies and whenever reflection is important (as compared to changes in the transmission amplitude). Several approaches do not include finite size terms, since they implicitly consider very large wave functions. The WKB approximation, the Oscillatory incident amplitude approach and the wavepacket analysis, for example, do not properly obtain finite size effects. On the other hand, our GF treatment, based on the Larmor clock, the generalization of the Time–modulated barrier approach and the Feynman path–integral treatments arrived to exact expressions. In order to see that these expressions are all equivalent one has to transform the derivative with respect to the average barrier potential, appearing in the Time–modulated barrier approach, into an energy derivative plus finite size terms. The same has to be done with the functional derivative with respect to the potential appearing in the Feynman path–integral techniques.

Finite size effects can be very important in mesoscopic systems with real leads with several transmitting modes–per current path. The energy appearing in the denominator of the finite size terms, Eqs. (47) and (67), corresponds in this case to the 'longitudinal' energy of each mode, and so there is a divergence whenever a new channel is open. In the exact expressions there are no divergences; the problematic contributions of the finite size terms is cancelled out by the terms with energy derivatives.

C Bopp's approach

Finally one of us (G.S.) wants to give some hints about one existing new alternative QM approach: Bopp's approach seems us to be not so well known in a broader circle of physicists, but we hope that readers will find it likewise interesting as we do, because within its framework there still is some freedom for the definition of time. Furthermore some critical problems with the wavepacket approach in mesoscopic systems and nanostructured materials hopefully can be avoided.

Bopp's QM [116] gives up the meaning of waves as some real dualistic appearance of quantum, and operates with manifest annihilation and creation processes instead. wave functions are only the expressions of the stochastic process and of our often incomplete knowledge of the events. But until now, his QM seems not to have found entrance in the theoretical treatment of tunnel processes.

Bopp's derivation, which he completed ten years ago on the basis of von Neumann's equation of the alternative, consequently starts with the undeniable (experimental) fact that in Q-physics particles can be created and annihilated. Therefore creation and annihilation must be considered as basic processes. Philosophically speaking, motion is not the fundamental driving force, but only occurs when a particle (a quantum) is annihilated in a certain point (of space) and an equal one is created in an infinitesimal neighboring point, and if this process is continuously going on during a certain time. Motions of that kind are compatible with the existence of some manifest creation and annihilation processes. Based on this idea, Q-physics can be derived from the above cited first principles.

According to this scenario, the nature of tunneling may be as follows. Annihilation in front of a tunneling barrier and *immediate* creation (only with different probabilities) either in front or behind the barrier (reflected or transmitted). Thus we cannot exclude that the time for creation on the right side (after tunneling) can possibly be infinitesimally small, perhaps even zero (and the same for creation on the left side in the reflected case), pretty independently of the barrier height and shape. Note that some problems like deformation and that of size of the wavepacket during such a process or the location of the center of gravity then have no further meaning, a fact which possibly simplifies analytic treatment of tunneling problems. But unfortunately two other difficulties with the tunneling problem arise. First, when approximating "classical" QM, Bopp's framework of QM claims that motion is creation in an *infinitesimally* neighboring point. The main question will be how to operationalize analytically the creation of a transmitted particle, *far* away beyond a tunnel barrier. Secondly, the introduction of a tunneling time.

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APPENDIX A: GREEN'S FUNCTION OF A LAYERED SYSTEM

We have been able to obtained the characteristic barrier interaction times in terms of the GF of the system, and more specifically as spatial integrals of the GF at coinciding coordinates, see for example Eq. (43). In the appendices we present a convenient model to calculate these integrals of the GF. We will closely follow Aronov *et al.* (1991), and introduce a general model for GF calculations of complex systems.

Let us consider that our system can be divided into $(N-1)$ layers, labelled $n = 1, ..., N-1$, which are placed between two semi-infinite media. The positions of the boundaries of the nth layer are given by y_n and y_{n+1}. We allow a possible discontinuity in the potential $V_n(y)$ at each boundary between two layers. This assumption does not imply a loss of generality, since we can reproduce any reasonable potential shape in the limit of an infinitely large number of layers, each of them of an infinitesimally small width.

We consider a plane wave incident from the left onto the boundary $y = y_1$ and we want to evaluate both the amplitude of the reflected wave and of the transmitted wave, propagating in the semiinfinite media for $y \geq y_N$.

In this method the GF is evaluated first for the case of a single boundary between two media. Then, the case of two boundaries is solved using the GF for one boundary. The problem is solved iteratively for $n+1$ boundaries, considering that the solution for n boundaries is known.

a One boundary

Let us first discuss the contact of two semi–infinite media, which will clearly show the spirit of the method. Assume that on the left of the boundary at y_1 $(y < y_1)$ the potential energy of the electron is $V_0(y)$, while on the right of the boundary $(y > y_1)$ the potential is $V_1(y)$. We suppose that the one–dimensional electron GF $G_n^{(0)}(y, y'; E)$ $(n = 0, 1)$ for each medium are known, when the media are infinite. In the following the energy parameter E will be omitted from the arguments of the GF. The GF is the solution of the following equation:

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial y^2} + V_n(y) - E\right] G_n^{(0)}(y, y'; E) = \delta(y - y') \tag{A1}$$

The upper index (l) will indicate the number of boundaries considered in the calculation of a given GF. In Eq. (A1), for example, the index is $l = 0$. The lower index of the GF labels the interval for which the GF is valid. The GF $G_0^{(1)}$ for the case when one interface is taken into account in the first medium can be expressed in the form

$$G_0^{(1)}(y, y') = G_0^{(0)}(y, y') + r_{01}\frac{G_0^{(0)}(y, y_1)\, G_0^{(0)}(y_1, y')}{G_0^{(0)}(y_1, y_1)}, \quad y, y' \leq y_1 \tag{A2}$$

The first term on the RHS corresponds to direct propagation between the two arguments of the GF, y and y', while the second term to propagation from y to the surface, reflection on the surface and propagation back to the point y'. r_{01} is the reflection amplitude of the electron propagating from region 0 into region 1, and we will calculate it below. A similar expression holds for the GF $G_1^{(1)}$ in the region on the right of the boundary $(y, y' \geq y_1)$:

$$G_1^{(1)}(y, y') = G_1^{(0)}(y, y') + r_{10}\frac{G_1^{(0)}(y, y_1)\, G_1^{(0)}(y_1, y')}{G_1^{(0)}(y_1, y_1)}. \tag{A3}$$

r_{10} is the reflection amplitude of the electron propagating from region 1 into region 0.

To calculate the quantities r_{01} and r_{10}, we have to enforce the condition of continuity for $G_0^{(1)}(y_1, y_1)$ and $G_1^{(1)}(y_1, y_1)$

$$G_0^{(1)}(y_1, y_1) = G_1^{(1)}(y_1, y_1) \tag{A4}$$

and the conservation of current at the boundary $y = y_1$

$$\frac{\partial}{\partial y}\left[G_0^{(1)}(y_1, y_1) - G_1^{(1)}(y_1, y_1)\right] = 0 \tag{A5}$$

where the derivative is taken over the two variables in the argument of the GF simultaneously. This condition may also be written in terms of derivatives with respect to the first argument of the GF only in the form:

$$\dot{G}_0^{(1)}(y_1 - 0, y_1) - \dot{G}_1^{(1)}(y_1 + 0, y_1) = \frac{2m}{\hbar^2}, \tag{A6}$$

Here the dot signifies the derivative with respect to the first argument, and it is necessary to distinguish between left-side and right-side derivatives of the GF due its discontinuity:

$$\dot{G}(y \mp 0, y) = \pm\frac{m}{\hbar^2} + \frac{1}{2}\frac{\partial}{\partial y}G(y, y) \tag{A7}$$

Solving Eqs. (A4) and (A6), we obtain the following expressions for the amplitudes of reflection $r_{01}$and r_{10}:

$$r_{01} = \frac{G_1^{(0)}\dot{G}_0^{(0)}(y_1 + 0, y_1) - G_0^{(0)}\dot{G}_1^{(0)}(y_1 + 0, y_1)}{G_1^{(0)}\dot{G}_0^{(0)}(y_1 - 0, y_1) - G_0^{(0)}\dot{G}_1^{(0)}(y_1 + 0, y_1)} \tag{A8}$$

$$r_{10} = \frac{G_1^{(0)}\dot{G}_0^{(0)}(y_1 - 0, y_1) - G_0^{(0)}\dot{G}_1^{(0)}(y_1 - 0, y_1)}{G_1^{(0)}\dot{G}_0^{(0)}(y_1 - 0, y_1) - G_0^{(0)}\dot{G}_1^{(0)}(y_1 + 0, y_1)} \tag{A9}$$

where we have used the notation $G_n^{(0)} \equiv G_n^{(0)}(y_1, y_1)$, for $n = 0, 1$.

We shall usually consider homogeneous media with constant potentials V_n of arbitrary strength. In this case we have

$$\frac{\partial}{\partial y} G_{0,1}^{(0)}(y, y) = 0 \tag{A10}$$

and the final expressions for r_{01} and r_{10}, Eqs. (A8) and (A9), become:

$$r_{01} = -r_{10} = \frac{G_1^{(0)} - G_0^{(0)}}{G_1^{(0)} + G_0^{(0)}} \tag{A11}$$

b Many boundaries

We can generalize the previous procedure by adding new boundaries and using each time the previously obtained GF as the starting point. In this way, we derive the new amplitudes of reflection of the electron on subsystems composed by many layers. Finally, the GF for the complete system at coinciding coordinates in the n-th layer (the left block containing n boundaries and the right block consisting of $(N-n)$ boundaries) is given by:

$$\begin{aligned} G_n^{(N)}(y, y) = G_n^{(0)}(y, y) \Big[& 1 + R_{n,n-1}^{(n)} R_{n,n+1}^{(-n+N)} \lambda_{n,n+1} \\ & + R_{n,n-1}^{(n)} e^{2i[\theta_n(y) - \theta_n(y_n)]} \\ & + R_{n,n+1}^{(-n+N)} e^{2i[\theta_n(y_{n+1}) - \theta_n(y)]} \Big] {D_N}^{-1}. \end{aligned} \tag{A12}$$

where the R are reflection amplitudes that we will define below, and D_N is a very important magnitude, containing all the information about the self-consistent problem of multiple reflections in the boundaries. This magnitude is called the characteristic determinant and can be expressed as the product:

$$D_N = D_N^0 \left\{ \prod_{n=1}^{N} \lambda_{n-1,n} (1 + r_{n,n-1})(1 + r_{n-1,n}) \right\}^{-1/2} \tag{A13}$$

We now define the different symbols appearing in this expression. The quantity $r_{n-1,n}$ ($r_{n,n-1}$) is the amplitude of reflection of the electron propagating from the region $n-1$ into n (n into $n-1$). In general the values of $r_{n,n-1}$ are model dependent and for a piece-wise constant potential is given by Eq. (A11), but replacing in the lower indices 0 by $n-1$ and 1 by n:

$$r_{n-1,n} = \frac{G_n^{(0)} - G_{n-1}^{(0)}}{G_n^{(0)} + G_{n-1}^{(0)}} \tag{A14}$$

The GF are the unperturbed GF evaluated with their two arguments at coinciding coordinates in y_n, $G_n^{(0)} \equiv G_n^{(0)}(y_n, y_n)$. The amplitude of reflection in the opposite direction satisfies $r_{n-1,n} = -r_{n,n-1}$. For a tight-binding model and a for set of delta functions, we have:

$$r_{n,n-1} = -\frac{V_n G_n^{(0)}}{1 + V_n G_n^{(0)}} \tag{A15}$$

and $r_{n-1,n} = r_{n,n-1}$, where V_n is the n-th diagonal energy in the tight-binding case, and the strength of the n-th delta function in the other case.

The factors $\lambda_{n-1,n}$ are defined, in general, as

$$\lambda_{n-1,n} = \exp\left(- \int_{y_{n-1}}^{y_n} \frac{2m}{\hbar^2} \frac{dy}{G_{n-1}^{(0)}(y, y)} \right), \tag{A16}$$

and the factor $\lambda_{0,1}$ is defined as equal to 1. For a piece-wise constant potential the previous expression reduces to:

$$\lambda_{n-1,n} = \exp\left(-\frac{2m}{\hbar^2} \frac{y_n - y_{n-1}}{G_{n-1}^{(0)}} \right), \tag{A17}$$

D_N^0 is the determinant of a tridiagonal matrix and satisfies the following recurrence relationship:

$$D_n^0 = A_n D_{n-1}^0 - B_n D_{n-2}^0 \tag{A18}$$

where

$$A_1 = 1; \qquad D_1^0 = 1; \qquad D_{-1}^0 = 0 \tag{A19}$$

and we have for $n > 1$:

$$A_n = 1 + \lambda_{n-1,n} \frac{r_{n-1,n}}{r_{n-2,n-1}} (1 + r_{n-2,n-1} + r_{n-1,n-2}), \tag{A20}$$

and

$$B_n = \lambda_{n-1,n} \frac{r_{n-1,n}}{r_{n-2,n-1}} (1 + r_{n-2,n-1})(1 + r_{n-1,n-2}) \tag{A21}$$

The generalized quantity $R_{n,n-1}^{(n)}$ is the amplitude of reflection from the left block, containing n boundaries (when the electron incides on this block from the right), and $R_{n,n+1}^{(-n+N)}$ is the amplitude of reflection from the right block, containing $N-n$ boundaries (when the electron incides on this block from the left). $\theta_n(y)$ is the phase factor defined in Eq. (38). The reflection amplitude $R_{n,n-1}^{(n)}$ may also be written in the form:

$$R_{n,n-1}^{(n)} = \frac{\tilde{D}_{n+1}^0}{D_n^0} \tag{A22}$$

where $\tilde{D}_{n+1}^0$ is given by

$$\begin{aligned} \tilde{D}_{n+1}^0 = & \frac{(1 + r_{n,n-1})(1 + r_{n-1,n})}{r_{n-1,n}} D_{n-1}^0 \\ & - \frac{(1 + r_{n,n-1} + r_{n-1,n})}{r_{n-1,n}} D_n^0. \end{aligned} \tag{A23}$$

$R^{(-n+N)}_{n,n+1}$ can also be written in a similar way to $R^{(n)}_{n,n-1}$. In the case of a symmetric barrier, we have $R^{(-n+N)}_{n,n+1} = R^{(n)}_{n,n-1}$.

To conclude this appendix let us note that the GF on the right side of the N-th boundary ($y, y' \geq y_N$) has the following form:

$$G^{(N)}_N(y,y') = G^{(0)}_N(y,y') + R^{(N)}_{N,N-1} \frac{G^{(0)}_N(y,y_N) G^{(0)}_N(y_N,y')}{G^{(0)}_0(y_N,y_N)} \tag{A24}$$

Here $R^{(N)}_{N,N-1}$ is the reflection amplitude of the whole system from the N-th boundary when the electron falls in from the right.

In a similar way, the GF on the left of the system ($y, y' \leq y_1$) can be written as:

$$G^{(N)}_0(y,y') = G^{(0)}_0(y,y') + R^{(N)}_{0,1} \frac{G^{(0)}_0(y,y_1) G^{(0)}_0(y_1,y')}{G^{(0)}_0(y_1,y_1)} \tag{A25}$$

where $R^{(N)}_{0,1}$ is the reflection amplitude of the system from the first boundary when the wave falls in from the left.

APPENDIX B: TRANSMISSION COEFFICIENT OF A LAYERED STRUCTURE

The method described on the previous appendix allows us to calculate any electronic property of a layered structure. In this appendix we show how to obtain the transmission coefficient of such a system from the characteristic determinant defined in appendix A.

By definition, the transmission coefficient is equal to the modulus square of the amplitude of the wave function at the right of the system when the electron incides on it from the left. Using the Fisher–Lee [117] relation between the scattering matrix and the GF, the transmission coefficient may be written as

$$T = \left[\left| G^{(0)}_0(y_1,y_1) \right| \left| G^{(0)}_N(y_N,y_N) \right| \right]^{-1} \left| G^N(y_1,y_N) \right|^2 \tag{B1}$$

where $G^N(y_1,y_N)$ is the GF of the electron in the layered structure with N boundaries.

In order to simplify the previous equation we rewrite the general expression for the GF $G(y,y')$ in terms of GF at coinciding coordinates $y = y'$, which can be done using Eq. (37):

$$G^{(N)}(y_1,y_N) = \left[\left| G^{(N)}(y_1,y_1) \right| \left| G^{(N)}(y_N,y_N) \right| \right]^{1/2} \exp i \left[\theta(y_N) - \theta(y_1) \right] \tag{B2}$$

where $\theta(y)$ is again the phase function defined by Eq. (38), so that

$$\theta(y_N) - \theta(y_1) = -\int_{y_1}^{y_N} \frac{m}{\hbar^2} \frac{dy}{G^{(N)}(y,y)} = -\sum_{n=1}^{N-1} \int_{y_n}^{y_{n+1}} \frac{m}{\hbar^2} \frac{dy}{G^{(N)}(y,y)}$$

We remember that the GF appearing in these two expressions $G^{(N)}_n(y,y')$, $G^{(N)}_N(y,y')$ and $G^{(N)}_0(y,y')$ are defined by Eqs. (A12), (A24) and (A25), respectively.

To calculate the integral appearing in Eq. (B3) we use the final expression for the GF obtained in the previous appendix, Eq. (A12). The spatial integral corresponding to layer n is equal to:

$$-\int_{y_n}^{y_{n+1}} \frac{m}{\hbar^2} \frac{dy}{G^{(N)}(y,y)} = \frac{m}{\hbar^2} \ln \frac{\lambda_{n,n+1}(1+R^{(n)}_{n,n+1})(1+R^{(-n+N)}_{n,n+1})}{(1+\lambda_{n,n+1}R^{(n)}_{n,n+1})(1+\lambda_{n,n+1}R^{(-n+N)}_{n,n+1})} \tag{B4}$$

Taking into account the previous expression, the definition of the determinant D^0_n, Eq. (A18), and the values of the generalized reflection amplitudes, Eq. (A22), we arrive at the following expression for the GF:

$$\begin{aligned} G^{(N)}(y_1,y_N) &= \Big\{ G^{(N)}_0(y_1,y_1) G^{(N)}_N(y_N,y_N) \\ &\times (1+R^{(N)}_0)(1+R^{(N)}_{N,N-1}) \\ &\times \prod_{n=1}^{N-1} \frac{\lambda_{n,n+1}(1+R^{(n)}_{n,n+1})(1+R^{(-n+N)}_{n,n+1})}{(1+\lambda_{n,n+1}R^{(n)}_{n,n+1})(1+\lambda_{n,n+1}R^{(-n+N)}_{n,n+1})} \Big\}^{1/2} \\ &= (D^0_N)^{-1} \Big(G^{(N)}_0(y_1,y_1) G^{(N)}_N(y_N,y_N) \\ &\times \prod_{n=1}^{N-1} (1+r_{n,n-1})(1+r_{n-1,n}) \Big)^{1/2} \end{aligned} \tag{B5}$$

Substituting this final expression for the GF $G^{(N)}(y_1,y_N)$, Eq. (B5), and the analogous expression for the complex conjugate of the GF, $\left[G^{(N)}(y_1,y_N)\right]^*$ in the expression for the transmission coefficient, Eq. (B1), we finally arrive at:

$$T = |D_N|^{-2} \tag{B6}$$

where D_N is the characteristic determinant, given by Eq. (A13). This is a general expression, valid for any model, which tell us that the transmission coefficient T of a system is inversely proportional to the characteristic determinant D_N.

APPENDIX C: INTEGRAL OF THE GREEN'S FUNCTION

We showed that the traversal time is proportional to the spatial integral of the GF at coinciding coordinates, which can be calculated exactly using the method developed in the previous appendices. Here we first prove the relations used in this article involving integrals of the GF, and secondly we obtain the exact expression of the

integral of the GF at coinciding coordinates in terms of the transmission and reflection coefficients.

Let us derive the equations appearing in the section on the dwell time. Our first aim is to obtain the spatial integral of the modulus square of the wave function. In order to do so, we start by trivially rewriting the wave function $\psi(y)$ in terms of derivatives with respect to energy

$$\psi(y) = (V(y) - E)\,\frac{\partial}{\partial E}\psi(y) - \frac{\partial}{\partial E}(V(y) - E)\,\psi(y) \quad \text{(C1)}$$

From here, and taking into account that the wave function is a solution of Schrödinger equation, we can express the square of the wave function in the form

$$\begin{aligned}\psi(y)^2 &= \frac{\hbar^2}{2m}\left(\psi''(y)\frac{\partial}{\partial E}\psi(y) - \psi(y)\frac{\partial}{\partial E}\psi''(y)\right) \quad \text{(C2)}\\ &\equiv \frac{\hbar^2}{2m}\frac{\partial}{\partial y}\left(\psi'(y)\frac{\partial}{\partial E}\psi(y) - \psi(y)\frac{\partial}{\partial E}\psi'(y)\right)\end{aligned}$$

Integrating both parts of this expression over y one gets

$$\begin{aligned}\int \psi(y)^2 dy &= -\frac{\hbar^2}{2m}\psi(y)^2\frac{\partial}{\partial E}\left(\frac{\psi'}{\psi}\right) \quad \text{(C3)}\\ &\equiv -\frac{\hbar^2}{2m}\psi(y)^2\frac{\partial}{\partial E}\left(\frac{\psi'\psi*}{|\psi|^2}\right)\end{aligned}$$

We now express this equation in terms of the GF, taking into account that the wave function is of the form

$$\psi = |\psi|\, e^{i\theta} \quad \text{(C4)}$$

where $\theta(y)$ is the phase function, Eq. (38). Eq. (C3) becomes:

$$\begin{aligned}&\int G(y,y)\; e^{2i\theta(y,E)} dy = -\frac{\hbar^2}{4m} G(y,y)\; e^{2i\theta(y)}\\ &\frac{\partial}{\partial E}\left[\left(G'(y,y) - \frac{2m}{\hbar^2}\right) G^{-1}(y,y)\right] \quad \text{(C5)}\end{aligned}$$

In a similar way, we have:

$$\begin{aligned}&\int G(y,y)\; e^{-2i\theta(y,E)} dy = -\frac{\hbar^2}{4m} G(y,y)\; e^{-2i\theta(y)}\\ &\frac{\partial}{\partial E}\left[\left(G'(y,y) + \frac{2m}{\hbar^2}\right) G^{-1}(y,y)\right] \quad \text{(C6)}\end{aligned}$$

We derived Eqs. (C5) and (C6) making use of the fact that the wave function $\psi(y)$ at energy E is related to the retarded Green function $G(y,y')$ of the system through the expression:

$$G(y,y') = \begin{cases} i\pi\nu(E)\psi(y)\psi^*(\,y') & \text{if } y > y' \\ i\pi\nu(E)\psi^*(y)\psi(y') & \text{if } y \le y' \end{cases} \quad \text{(C7)}$$

where $\nu(E)$ is the density of states per unit energy and per unit length. Note that at coinciding coordinates, this expression reduces to the well known result $G(y,y) = i\nu(E)|\psi(y)|^2$. From Eq. (C7) we can obtain the left-side and right-side derivatives of the GF with respect to coordinates, which have to be distinguished due to discontinuity:

$$\dot{G}(y \mp 0, y) = \pm\frac{m}{\hbar^2} + \frac{1}{2}G'(y,y) \quad \text{(C8)}$$

Here the dot signifies the derivative with respect to the first argument, keeping fixed the second argument and the energy.

Using the expressions for the wave function, Eq. (C1), and for its square, Eq. (C2), we can represent $|\psi(y)|^2$ in the following form

$$\begin{aligned}|\psi(y)|^2 = \frac{\hbar^2}{4m}\frac{\partial}{\partial y}\Bigg\{&\left(\psi'(y)\frac{\partial}{\partial E}\psi^*(y) + \psi^{*\prime}(y)\frac{\partial}{\partial E}\psi(y)\right)\\ &- \left(\psi(y)\frac{\partial}{\partial E}\psi^{*\prime}(y) + \psi^*(y)\frac{\partial}{\partial E}\psi'(y)\right)\Bigg\} \quad \text{(C9)}\end{aligned}$$

Integrating both parts of this expression over y one gets

$$\begin{aligned}\int |\psi(y)|^2\, dy = -\frac{\hbar^2}{4m}\Bigg\{&\psi^{*2}(y)\frac{\partial}{\partial E}\left(\frac{\psi'(y)\psi(y)}{|\psi(y)|^2}\right)\\ &+ \psi^2(y)\frac{\partial}{\partial E}\left(\frac{\psi^{*\prime}(y)\psi^*(y)}{|\psi(y)|^2}\right)\Bigg\} \quad \text{(C10)}\end{aligned}$$

A straightforward calculation, using Eqs. (C4), (C7) and (C8), leads to

$$\int G(y,y)dy = i\frac{\partial}{\partial E}\theta(y) - \frac{\hbar^2}{4m}G(y,y)\frac{\partial}{\partial E}\left(\frac{G'(y,y)}{G(y,y)}\right) \quad \text{(C11)}$$

This completes the deduction of the set of useful integrals which were used in this article.

Now we can go a step further and calculate the spatial integral of the GF at coinciding coordinates, given by Eq. (C11), over the region $[0, L]$, which appears in the calculation of the traversal time, Eq. (43). Without loss of generality we will discuss the case when the potential $V(y)$ is zero outside the interval $[0, L]$. In this case the GF's outside the barrier are $G_0^{(0)}(0,0) = G_N^{(0)}(0,0) = im/k\hbar^2$.

The expression for the GF on the left of the barrier, given by Eq. (A25), when evaluated at $y = y' = 0$ reduces to:

$$G(0,0) = G_0(0,0)\,(1 + r) \quad \text{(C12)}$$

where we have relabeled the total reflection amplitude from the left as $r \equiv R_{0,1}^{(N)}$. Analogously, the expression for the GF on the right of the barrier, Eq. (A24), when evaluated at $y = y' = L$ becomes:

$$G(L,L) = G_0(L,L)\,(1 + r') \quad \text{(C13)}$$

where $r' \equiv R_{N,N-1}^{(N)}$ is the total reflection amplitude from the right. The derivative of the GF $G'(y,y)$ at the origin is equal to

$$G'(0,0) = \frac{2mr}{\hbar^2} \quad \text{(C14)}$$

while its derivative at $y = y' = L$ is

$$G'(L,L) = -\frac{2mr'}{\hbar^2}. \tag{C15}$$

Making use of the expressions of the GF at 0 and at L, Eqs. (C12) and (C13), and of the derivative of the GF at 0 and at L, Eqs. (C14) and (C15),we can rewrite the integral of the GF, Eq. (C11), as

$$\int_0^L G(y,y;E)\, dy = i\frac{\partial}{\partial E}\left[\theta(L) - \theta(0)\right] \tag{C16}$$
$$+ \frac{\partial}{\partial E}\ln(1+r)(1+r') + \frac{1}{4E}(r+r')$$

The next step to get the final answer is to calculate the first bracket in Eq. (C16). It is straightforward to show, using Eqs. (B4) and (B5), that the bracket can be represented in the form:

$$i\left[\theta(L) - \theta(0)\right] = \ln\frac{t}{(1+r)(1+r')} \tag{C17}$$

Substituting this expression in Eq. (C16) we finally obtain for the spatial integral of the GF, and so for the traversal time, Eq. (43), the following expression:

$$\int_0^L G(y,y;E)\, dy = \frac{\partial \ln t}{\partial E} + \frac{1}{4E}(r+r'). \tag{C18}$$

In the rest of this Appendix, starting from the explicit expression for the integral of $G_n^{(N)}(y,y)$ in each layer, given by Eq. (A12), we show that the sum of the contributions of all the layers yields also the result previously obtained, Eq. (C18). For a piece-wise constant potential, the integral over a layer of the GF, as was first done by Aronov *et al* (1991), is:

$$\int_{y_n}^{y_{n+1}} G_n^{(N)}(y,y)\, dy = \frac{\partial \ln t}{\partial V_n}, \tag{C19}$$

where V_n is the potential energy of electron in the n-th subsystem and t is the transmission amplitude of the whole system. We could write the total integral of the GF as a sum of terms of the form given by Eq. (C19):

$$\int_0^L G^{(N)}(y,y)\, dy = \tag{C20}$$
$$\sum_{n=1}^{N-1}\int_{y_n}^{y_{n+1}} G_n^{(N)}(y,y)\, dy = \sum_{n=1}^{N-1}\frac{\partial \ln t}{\partial V_n},$$

A similar expression to this Eq. (C20) was found, on a different context, by García-Moliner and Flores (1979) in terms of surface GF. In the $N \to \infty$ limit (keeping L fixed) and converting the summation into an integral, Eq. (C20) becomes

$$\int_0^L G^{(N)}(y,y)\, dy = \int_0^L \frac{\delta \ln t}{\delta V(y)}\, dy, \tag{C21}$$

where $\delta/\delta V(y)$ is a functional derivative. This is the result of Sokolovski and Baskin (1987).

As was shown by Leavens and Aers (1987) the functional derivative with respect to the potential can be replaced by the derivative with respect to the average height of the potential $\overline{V}$, keeping the spatial variation of the potential fixed. We thus obtain

$$\int_0^L \frac{\delta \ln t}{\delta V(y)}\, dy = \frac{\delta \ln t}{\delta \overline{V}}. \tag{C22}$$

We would like to remember that we have shown that the integral of the GF at coinciding coordinates, equal to Eq. (C22) can also be written exactly in terms of derivatives with respect to energy, plus a correction term, expression (C18).

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