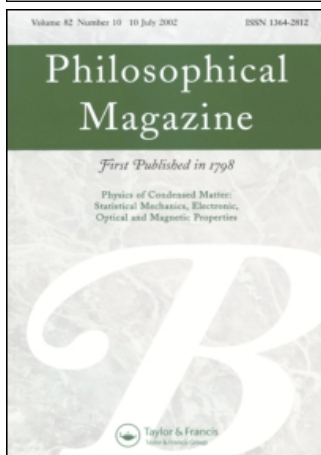


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Green's function formulation of the traversal time and nature of the complex time

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ABSTRACT

We develop a Green's function formalism and with it we are able to obtain close expressions for the tunnelling and for the reflection times. For each problem, there appear two characteristic times which correspond to the real and imaginary parts of the integral of the Green's function at coinciding coordinates. The time related to the imaginary part represents the minimum uncertainty of the measurement. A strong analogy between the results of the different existing approaches is established, and we show that their main differences are due to finite-size effects.

§1. INTRODUCTION

The question of the time spent by a particle in a given region of space is not new, but it has recently attracted much interest (see Hauge and Støvneng (1989), Leavens and Aers (1990), Landauer and Martin (1994) and Gasparian *et al.* (1999a, b), and references therein). The problem has been approached from many different points of view, and there exists a huge literature on the tunnelling problem of electrons through a barrier, although tunnelling times have continued to be controversial even until now. There is no clear consensus about simple expressions for the time in quantum mechanics, where there is not a Hermitian operator associated with it (Landauer and Martin 1994).

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 (Baz' 1967, Rybachenko 1967, Büttiker 1983). Gasparian *et al.* (1995) have developed similar procedures for electromagnetic waves. They proposed a clock based on the Faraday effect to measure the interaction time of electromagnetic waves in a slab. Another approach is to calculate the traversal time of a particle through a barrier by following the behaviour of a wave packet and to determine the delay due to the structure of the region. Martin and Landauer (1992) used this approach to study the traversal

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time of classical evanescent electromagnetic waves, and Ruiz *et al.* (1997) analysed the behaviour of these waves in the optical gap of a periodic structure.

We first study the Larmor clock approach to tunnelling time, and we then re-express the results in terms of Green's functions (GFs). For one-dimensional (1D) systems we obtained closed expressions for the traversal and reflection times (equations (23) and (24)), in terms of partial derivatives of the transmission and reflection amplitudes with respect to energy. The 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. We shall try to give a coherent explanation of these differences, concentrating mainly on the meaning of the two components of the complex time.

§ 2. LARMOR CLOCK APPROACH

Baz' (1967) proposed the use of the Larmor precession as a clock ticking off the time spent by a spin $\frac{1}{2}$ 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. 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 stays 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

$$\omega_L = \frac{2\mu B}{\hbar}. \quad (1)$$

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 θ_\perp in the x - y plane, perpendicular to the magnetic field, between the initial and final polarizations is assumed to be given, to lowest order in the field, by the Larmor frequency ω_L multiplied by the time τ_y spent by the particle in the sphere

$$\theta_\perp = \omega_L \tau_y. \quad (2)$$

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

Rybachenko (1967), following the method of Baz', considered the simpler problem of the interaction time of particles with a 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 wavefunction, the following result was found for the expectation value of the spin components of transmitted particles, to lowest order in the field \mathbf{B} :

$$\langle S_x \rangle \approx \frac{\hbar}{2}, \quad (3)$$

$$\langle S_y \rangle \approx -\frac{\hbar}{2} \omega_L \tau_y, \quad (4)$$

where τ_y is a characteristic interaction time given by

$$\tau_y = \frac{\hbar k}{V_0 \xi}, \quad (5)$$

and ξ is the inverse decay length in the rectangular barrier given by

$$\xi = (k_0^2 - k^2)^{1/2}, \quad (6)$$

with $k_0 = (2mV_0)^{1/2}/\hbar$. Here we have assumed that the direction of the field and the direction of propagation of the particles are the same as defined at the beginning of the section. This means that the spin, to first order in the field, remains in the x - y 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 (1962) analysing the tunnelling of a wave packet through a rectangular potential barrier. Thus so-called 'superluminal velocities' can be measured in some cases such as in experiments where electromagnetic waves pass through a barrier (Enders and Nimtz 1992, Mugnai *et al.* 1994) or through an optical gap (Steinberg *et al.* 1993, Spielman *et al.* 1994, Balcou and Dutriaux 1997). Recently the possibility of observing 'superluminal' behaviour in the propagation of localized microwaves have been demonstrated by Mugnai *et al.* (2000). Gain-assisted 'superluminal' light propagation was experimentally realized by Wang *et al.* (2000) in atomic caesium gas.

Büttiker (1983) presented a detailed analysis of the Larmor clock for the case of a 1D rectangular barrier. His conclusion was 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 (the Zeeman effect). This means that a particle tunnelling through a barrier in a magnetic field performs not only 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 $\frac{1}{2}$ and equal to $-\hbar/2$ with probability $\frac{1}{2}$. Outside the barrier the particles have an energy E independent of the spin, but in the barrier the energy differs by the Zeeman contribution $\pm \hbar \omega_L/2$, giving rise to a different exponential decay of the wave function depending on its spin component along the direction of the magnetic field.

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

$$\tau^{\text{BL}} = [(\tau_y^{\text{BL}})^2 + (\tau_z^{\text{BL}})^2]^{1/2} = \frac{(\theta_\perp^2 + \theta_\parallel^2)^{1/2}}{\omega_L}. \quad (7)$$

Here θ_\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 and spin down 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 tunnelling, it is a general definition which applies for the traversal time of a particle through any given region of space.

§ 3. FORMALISM IN TERMS OF GREEN'S FUNCTIONS

Let us now derive a general expression for the BL traversal (and reflection) time using the GF method developed by Gasparian and Pollak (1993) and Gasparian *et al.* (1995b). We shall consider a 1D system with an arbitrary potential $V(y)$ confined to a finite segment $0 < y < L$. We shall call this region ‘the barrier’, and we shall assume that scattering in it is 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.

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

$$\hat{\Psi}(y) = \begin{pmatrix} \Psi_1 \\ \Psi_2 \end{pmatrix} \quad (8)$$

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 wavefunction before entering the barrier is given by

$$\hat{\Psi}(y) = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \exp(iky). \quad (9)$$

We are considering a plane wave for the wavefunction, but our results are valid for any wave packet provided that it is much longer than the size L of the barrier.

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

$$\left(-\frac{\hbar^2}{2m} \frac{d^2}{dy^2} + V(y) - E \right) \hat{\Psi}(y) = -\boldsymbol{\mu} \cdot \mathbf{B} \hat{\Psi}(y) = -\mu B \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \hat{\Psi}(y). \quad (10)$$

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

$$\boldsymbol{\mu} \cdot \mathbf{B} = 2\mu S_z B = \mu \sigma_z B = \mu B \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad (11)$$

where σ_z is a Pauli matrix.

The problem is solved by perturbation theory. To the lowest order in B , the spinor $\hat{\Psi}(L)$ of the electron on the right end of the barrier is given by (Gasparian and Pollak 1993):

$$\hat{\Psi}(L) = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \psi(L) + \frac{e\hbar B}{2mc} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \int_0^L \psi(y) G(y, L) dy. \quad (12)$$

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 wavefunction can be written in terms of the GF of the system as

$$\psi(y) = \exp(iky) - \int_0^L G(y, y') V(y') \exp(iky') dy', \quad (13)$$

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

$$G(y, y') = G_0(y, y') + \int_0^L G_0(y, y'') V(y'') G(y'', y') dy'', \quad (14)$$

where $G_0(y, y') = i(m/k\hbar^2) \exp(ik|y - y'|)$ 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.

We shall 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 ,

$$\begin{aligned} \langle S_z \rangle &= \frac{\hbar}{2} \langle \hat{\Psi}(L) | \sigma_z | \hat{\Psi}(L) \rangle \\ &= -\frac{e\hbar^2 B}{mc} \operatorname{Re} \left(\psi^*(L) \int_0^L \psi(y) G(L, y) dy \right). \end{aligned} \quad (15)$$

We want to express the wavefunction $\psi(y)$ 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 wavefunction and the GF of a 1D system:

$$\psi(y) = -\frac{i\hbar^2 k}{m} G(0, y). \quad (16)$$

For 1D systems also, we can further simplify the problem by writing the general expression for the GF, namely $G(y, y')$, in terms of its own expression at coinciding coordinates $y = y'$ (Aronov *et al.* 1991):

$$\begin{aligned} G(y, y') &= [G(y, y) G(y', y')]^{1/2} \exp \left(- \int_{\min(y, y')}^{\max(y, y')} \frac{m}{\hbar^2} \frac{dy_1}{G(y_1, y_1)} \right) \\ &= [G(y, y) G(y', y')]^{1/2} \exp [i|\theta(y) - \theta(y')|], \end{aligned} \quad (17)$$

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

$$\theta(y) = \int_0^y \frac{im}{\hbar^2} \frac{dy'}{G(y', y')}. \quad (18)$$

Finally one finds the spin component along the direction of the magnetic field:

$$\langle S_z \rangle = \frac{e\hbar^2 B}{mc} |\psi(L)|^2 \operatorname{Re} \left(\int_0^L G(y, y) dy \right). \quad (19)$$

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

$$\langle S_y \rangle = -\frac{e\hbar^2 B}{mc} |\psi(L)|^2 \operatorname{Im} \left(\int_0^L G(y, y) dy \right). \quad (20)$$

and

$$\langle S_x \rangle = \frac{\hbar}{2} |\psi(L)|^2 \left(1 - \frac{1}{2} \left| \frac{2e\hbar B}{mc} \int_0^L G(y, y) dy \right|^2 \right). \quad (21)$$

The BL characteristic traversal times for the z and y directions are proportional to the corresponding spin components (equations (20) and (21)), and we finally arrive at:

$$\begin{aligned} \tau_z^{\text{BL}} &= \hbar \operatorname{Re} \left(\int_0^L G(y, y) dy \right), \\ \tau_y^{\text{BL}} &= \hbar \operatorname{Im} \left(\int_0^L G(y, y) dy \right). \end{aligned} \quad (22)$$

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

$$\tau = \tau_z^{\text{BL}} + i\tau_y^{\text{BL}} = \hbar \int_0^L G(y, y) dy = \hbar \left[\frac{\partial(\ln t)}{\partial E} + \frac{r + r'}{4E} \right]. \quad (23)$$

This is a general expression, independent of the model considered, and t and r are the transmission and reflection amplitudes from the finite system. r' is the reflection amplitude of the electron from the whole system, when it falls in from the right. It is also valid for electromagnetic waves (Ruiz *et al.*, 1997).

The term proportional to $\partial(\ln t)/\partial E$ in equation (23) 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 of the order of the wavelength λ over the length of the system L , that is $O(\lambda/L)$. Thus, it becomes important for low energies and/or short systems. We believe that equation (23) is exact for wave packets larger than the system size and adequately incorporates finite-(sample)-size effects, which correspond to the terms that which are not proportional to derivatives with respect to energy. 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 (equation (23)) 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 are cancelled out by the terms with energy derivatives (Gasparian *et al.* 1996).

Several approaches do not include finite size terms, since they implicitly consider very large wavefunctions. For instance, the Wentzel–Kramers–Brillouin approximation (Büttiker and Landauer 1985), the oscillatory incident amplitude approach (Büttiker and Landauer 1986, Leavens and Aers 1987) and the wave-packet analysis (for example Hauge and Støvneng (1989) and Landauer and Martin (1994)) do not properly obtain finite-size effects. On the other hand, our GF treatment, the generalization of the time-modulated barrier approach (Jauho and Jonson 1989) and the Feynman path-integral treatments (Sokolovski and Baskin 1987) arrived at 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.

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 τ_R from an arbitrary 1D barrier can be calculated in the same way as we have done for transmitted waves. We shall use the subscript R to indicate that the magnitude corresponds to reflection, and we understand that similar magnitudes related to transmission will have no equivalent subscript. Proceeding as above, we find that the two characteristic reflection times $\tau_{y,R}^{BL}$ and $\tau_{z,R}^{BL}$ can be written as the complex reflection time τ_R , in analogy with the complex traversal time τ given in equation (23):

$$\tau_R = \tau_{z,R}^{BL} + i\tau_{y,R}^{BL} \equiv \hbar \left(\frac{\partial \ln r}{\partial E} - \frac{1}{4Er} (1 - r^2 - t^2) \right). \quad (24)$$

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 and so the characteristic times for transmission and reflection corresponding to the direction of propagation are equal:

$$\tau_y^{BL} = \tau_{y,R}^{BL}, \quad (25)$$

as immediately follows from equations (23) and (24) (see also the review article by Hauge and Støvneng (1989)). For the special case of a rectangular barrier, equation (25) was first found by Büttiker (1983). Comparison of the equations (23) and (24) shows that, for an asymmetric barrier, equation (25) breaks down (Leavens and Aers 1987).

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 1983, Sokolovski and Baskin 1987):

$$R\tau_{z,R}^{BL} + T\tau_z^{BL} = 0, \quad (26)$$

which can be checked directly using equations (23) and (24). T and $R = 1 - T$ are the transmission and reflection probabilities respectively.

To close this section note that the GF method was generalized to the problem of an electron escaping from a 1D disordered region by Lopez Villanueva and Gasparian (1999), based on the local version of the Larmor clock, that is when an infinitesimal magnetic field B is localized inside the barrier (Leavens and Aers, 1988). It was shown that, in the case of a quantum well surrounded by right and left arbitrary barriers, and an additional weak magnetic field \mathbf{B} oriented in the z direction and finite only in the interval $[y_0, L]$, the coordinate-dependent complex escape time $\tau_{r,y}^{\text{esc}}(y_0, L; E)$ has two components, that is both a precession and a rotation of spin. For instance, the y component can be defined as

$$\begin{aligned}\tau_{r,y}^{\text{esc}}(y_0, L; E) &= \text{Im} \left(\int_{y_0}^L G(y, y; E) dy \right) \\ &= \text{Im} \left[\frac{\partial(\ln t_r)}{\partial E} + \frac{\tilde{r}_r + r'}{4E} + \frac{1}{2}(1 - \tilde{r}_r) \frac{\partial}{\partial E} \ln \left(\frac{1 - \tilde{r}_r}{1 + \tilde{r}_r} \right) \right].\end{aligned}\quad (27)$$

Here $t_r \equiv t_r(y_0, L; E)$ is the complex amplitude of transmission only through the right barrier (see equation (23)). $\tilde{r}_r \equiv \tilde{r}_r(y_0, L; E)$ has a slightly different meaning; the tilde signifies that the given quantity is calculated in the presence of the left and right barriers (Aronov *et al.*, 1991). Thus \tilde{r}_r is the complex amplitude of reflection from the right barrier in the presence of the left barrier, when the electron falls in this barrier from the left.

Note that the integral in equation (27) runs from y_0 to L , instead of from 0 to L , as occurred in the case of a free incident electron and obviously, for $y_0 = 0$, coincides with equation (23).

§ 4. COMPLEX TIME AND UNCERTAINTY

Although the tunnelling time must be a real time, the concept of complex time in the theory of the traversal time problem of electrons and of classical electromagnetic waves has arisen in many approaches (see Martin (1996), and references therein). Pollak and Miller (1984), while studying the average tunnelling time in classical chemical systems, arrived at the concept of an imaginary time through the flux-flux correlation function. Leavens and Aers (1987) also arrived at the idea of a complex barrier interaction time, by studying the shape distortion of the transmitted wave by the barrier using the oscillatory incident amplitude approach. 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 Feynman path-integral approach the concept of a complex time also arises naturally. Sokolovski and Baskin (1987), using this kinematic approach to quantum mechanics found the following complex time:

$$\tau = i\hbar \int_0^L \frac{\delta(\ln t)}{\delta V(y)} dy, \quad (28)$$

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

The result in equation (28) is strictly equivalent to equation (23) for the integrated density of states, and so we can emphasize that this coincidence is quite natural, because in the tunnelling time problem we always deal with an *open* and *finite* system. The functional derivative with respect to the potential appearing in equation (28) is equivalent to a derivative with respect to energy plus a correction term proportional to the reflection coefficient.

The optical analogue of the Larmor clock for classical electromagnetic waves based on the Faraday effect leads us also to a complex time (Gasparian *et al.* 1995a). The two time components are calculated using the expression for the complex traversal time in terms of derivatives with respect to frequency ω (Ruiz *et al.* 1997):

$$\tau_T(\omega) = \tau_1(\omega) - i\tau_2(\omega) = -i \left(\frac{\partial(\ln t)}{\partial \omega} - \frac{r}{\omega} \right). \quad (29)$$

Gasparian *et al.* (1999a,b) have shown that the two components $\tau_1(\omega)$ and $\tau_2(\omega)$ of the complex traversal time $\tau(\omega)$ are not independent quantities but are connected by Kramers–Kronig relations. The validity of the Kramers–Kronig relations is a direct result of the causal nature of physical systems by which the response to a stimulus never precedes the stimulus.

Many experimental and theoretical investigators analyse only the behaviour of the $\tau_1(\omega)$ component of evanescent modes, which is not necessarily Einstein causal (Nimtz 1999), and obtain in this way superluminal velocities. The signal or wave packet spends a very short time in the evanescent region, and so the delay time is smaller than the crossing time at the vacuum speed of light. From extensive numerical simulations we have found that the component τ_2 is directly connected to the minimum possible error in the traversal time. Let us explain this in more detail. If we start with a very long wave packet and obtain a very short traversal time, there is no problem with causality since the uncertainty in the measurement is much larger than the traversal time itself. The question is how short can we make the initial wave packet and still have a very short traversal time. The answer to this question lies in the imaginary component of time τ_2 ; we obtain very short times for packets larger than τ_2 multiplied by the group velocity. As this component is large in the situations where causality seemed to be violated, the possible paradox is solved. We believe that the solution to this paradox is via uncertainty and not because the relevant time is the modulus of the complex time.

The association of τ_2 with the uncertainty in the time not only arises from our numerical results but also can be deduced from the formulation of the problem itself. This is easier to appreciate in the case of electromagnetic waves where we start with linearly polarized waves and measure the angle of rotation, proportional to τ_1 , and the ellipticity, proportional to τ_2 . The amount of ellipticity represents an uncertainty in the measurement of the rotation angle. A similar situation occurs for electrons. We have to measure the component of spin along the y axis, which is proportional to τ_1 . We cannot measure simultaneously the other component, but we know that the average value of the other component, owing to the Zeeman effect, produces an uncertainty in the expectation value of τ_1 .

§ 5. CONCLUSIONS

We have discussed the topic of tunnelling time in mesoscopic systems, particularly in 1D systems with an arbitrarily shaped potential. All the existing different approaches can be consistently formulated in terms of GFs, and their main differences can be fairly well understood.

As regards the complex nature of time our conclusion is the following. It is clear that there are two characteristic times to describe the tunnelling 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. We propose that the quantity that is always measured is the real component of time τ_1 , while the uncertainty in the traversal time, as well as the minimum size of the wave packet where ultrashort times can be achieved, is controlled by the imaginary component τ_2 .

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