

Compact formula for the density of states in a quantum well

G. Iannaccone* and B. Pellegrini

*Dipartimento di Ingegneria dell'Informazione: Elettronica, Informatica e Telecomunicazioni, Università degli studi di Pisa,
Via Diotisalvi 2, I-56126 Pisa, Italy*

(Received 11 May 1995)

In this paper we derive a formula for the density of states in the presence of inelastic scattering in the quantum well of a double-barrier structure as a function of a characteristic time of the motion of electrons (namely, the round-trip time in the well) and of transmission probabilities for the whole structure and for each barrier. In the model we use, the scattering processes due to phonons, impurities, and interface roughness are taken into account by a unique phenomenological parameter, the mean-free path, which plays the role of a relaxation length. We also show that, for lower rates of incoherent processes, the derived formula reduces to the one obtained by means of the Breit-Wigner formalism.

I. INTRODUCTION

The density of states is one of the most important quantities for the study of equilibrium and transport properties of quantum effect devices. A recently derived formula¹ establishes a simple general relation between the density of states in a mesoscopic system and the dwell times for each incoming channel connecting the system to the external world.

In this paper we apply that result to the quantum well of a double-barrier resonant tunneling diode. Moreover, in order to get closer to real systems and experimental results, we consider the effects of inelastic processes taking place in the well, which are not accounted for in the general relation of Ref. 1.

We obtain a very compact formula connecting the density of states in the well to a characteristic time of electron motion in double-barrier structures, i.e., the time an electron takes to complete a round trip of the well, and to the transmission probabilities for the whole structure and for each barrier.

In the literature the density of states in the well is usually obtained using Breit-Wigner formulas,²⁻⁴ which lead to very simple and compact expressions. Dissipation can be easily accounted for by introducing a partial resonance width for all the inelastic processes.⁴⁻⁶ However, for Breit-Wigner formulas to hold true, it is necessary that all the partial resonance widths be much smaller than the separation between the resonant energy levels, and between each level and the top and bottom of the potential well. This condition establishes an upper limit on the rate of incoherent processes for the applicability of the Breit-Wigner formulas.

On the contrary, our model is valid even when coherence is completely destroyed. Scattering with phonons, impurities, and interface roughness is accounted for by a unique phenomenological parameter l , the mean-free path, a concept which is well established in solid state physics.⁷

We assume that an electron traversing an infinitesimal length dx of the one-dimensional device structure experiences a collision with probability dx/l , and that electrons emerge from collisions with an equilibrium distribution function in a state with completely random phase. This means, for instance, that the square amplitude of a plane wave func-

tion of wave vector k attenuates exponentially as it propagates along the x axis, with a characteristic length equal to l . It is a situation very similar to an electromagnetic wave propagating in a dissipative medium. The difference is that the number of electrons has to be conserved; therefore, electrons which seem to have disappeared have actually made a transition to a different state, with a phase completely uncorrelated, so that there is no quantum interference between these electrons and those that have not undergone an incoherent process. In this model, all collision processes are effective in randomizing phase and energy, and we do not make any difference between the effects of elastic scattering (due to impurities and interface roughness) and inelastic scattering (with phonons, for instance). A more sophisticated model should take into account these differences, and, as a minor improvement, phase randomization and energy relaxation could be split using a different characteristic length for each process.

Büttiker⁴ proposed a model for the inclusion of incoherent processes which is similar to the one we use. There is an inelastic scatterer in the well modeled by an extra branch leading away from the conductor to an extra reservoir, which does not draw net current, but permits phase randomizing events. Anyway, such a model is valid for very small differences between electrode chemical potentials and/or when energy relaxation is not accounted for.⁸ In the model by Knäbchen,⁹ the inelastic scattering probability ϵ for an electron traversing the well introduced by Büttiker is simply substituted by $\exp(-w/l)$, where w is the well width and l the mean-free path.

In our model scattering is spread over the whole region, and not concentrated in a single point, and any potential profile can be considered. No additional condition is required to obtain formula (22) for the density of states. The hypothesis of smooth potential in the well is imposed in order to obtain the compact formula (28). The importance of the energy relaxation mechanism will be shown elsewhere.¹⁰

As we shall show in Sec. III, we use in our formula a characteristic time of electron motion in the well defined on the basis of Larmor times for transmission and reflection.¹¹⁻¹⁸ The tunneling time problem is the subject of a long-standing controversy: while the dwell time¹³ is widely

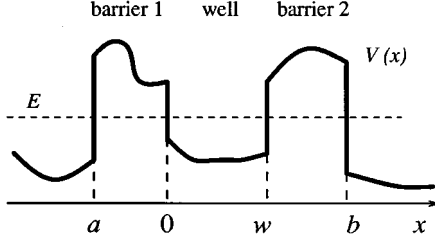


FIG. 1. The one-dimensional potential $V(x)$ defines the two barriers $[(a,0)$ and $(w,b)]$ and the well $(0,w)$.

accepted in the scientific community, there is no consensus on the actual time spent in a region by transmitted and reflected particles,^{15,19,20} due to the fact that there is no operator for time in quantum mechanics (therefore we cannot perform a direct measurement of time) and that electrons do not follow actual trajectories in the Copenhagen interpretation.²² The Larmor times are obtained as the result of an indirect measurement: a weak perturbation is applied to the region of interest (i.e., a magnetic field, a real potential, or an imaginary potential) and some variation in the properties of transmitted and reflected particles is measured (spin precession, phase rotation, or particle absorption, respectively).^{12–18,21} What is controversial about Larmor times is the interpretation of such results of an indirect measurement as the “actual” times spent in the considered region. However, this point is not relevant to the aim of the present work, where we are just interested in deriving a relation between the Larmor times and the density of states in a quantum well.

Our paper is organized as follows: in Sec. II we calculate the transmission and reflection probabilities by using the transfer matrix technique; in Sec. III we derive a formula for the density of states in the case of completely coherent transport. A completely analogous formula which takes into account the effects of dissipation is obtained in Sec. IV, and is shown to reduce to the Breit-Wigner formulas for lower rates of incoherent processes in Sec. V. A summary ends the paper.

II. TRANSMISSION AND REFLECTION PROBABILITIES FOR DOUBLE BARRIERS

Let us refer to the case sketched in Fig. 1: the one-dimensional potential energy profile $V(x)$ defines the first barrier $(a,0)$, the well region $(0,w)$, and the second barrier (w,b) . Let us also introduce the wave vector $k(x) \equiv [2m(E - V(x))]^{1/2}/\hbar$ for all x where $V(x) < E$, where m is the electron effective mass in the material of the well, and \hbar is the reduced Planck's constant.

We can calculate the total transmission and reflection coefficients by using the transfer matrix technique.^{23–26} In the assumption of coherent transmission through each single barrier, the transfer matrix M_1 for the first barrier satisfies all the properties listed in Ref. 23 and has the form

$$M_1 = \begin{bmatrix} 1/t_1^{(l)} & r_1^{(l)*}/t_1^{(l)*} \\ r_1^{(l)}/t_1^{(l)} & 1/t_1^{(l)*} \end{bmatrix}, \quad (1)$$

where $t_1^{(l)}$ and $r_1^{(l)}$ are the transmission and reflection coefficients, respectively, for a plane wave coming from the left

electrode, with wave vector $k_{1l} \equiv k(a)$. The corresponding coefficients $t_1^{(r)}$ and $r_1^{(r)}$ for a particle coming from the right with wave vector $k_{1r} \equiv k(0)$ are $t_1^{(r)} = t_1^{(l)} k_{1r}/k_{1l}$ and $r_1^{(r)} = -r_1^{(l)*} t_1^{(l)}/t_1^{(l)*}$. Moreover, if $T_1 = |t_1^{(r)}|^2 k_{1r}/k_{1l} = |t_1^{(r)}|^2 k_{1l}/k_{1r}$ is the transmission probability, and $R_1 = |r_1^{(l)}|^2 = |r_1^{(r)}|^2$ is the reflection probability, we have $R_1 + T_1 = 1$, i.e., the continuity equation for the probability density current holds true. The same considerations apply to the second barrier and its transfer matrix M_2 , provided that we define $k_{2l} \equiv k(w)$, $k_{2r} \equiv k(b)$ and change all the subscripts 1 into 2.

In the well region, dissipative processes are accounted for by means of the mean-free path l ; that is, the intensity of a plane wave of wave vector k' has a decay length equal to l . As a consequence, the probability density current for a given wave function is not conserved. The effect of l is taken into account by using a complex wave vector $k'_i = k' + i/2l$: a plane wave of wave vector k'_i along the x axis has the form $\exp(ik'_i x) = \exp(ik'x) \exp(-x/2l)$; therefore its square modulus decays as $\exp(-x/l)$.

The multistep potential approximation²⁷ can be used to obtain the transfer matrix M_w of the well, provided that the complex wave vector $k_i(x) = k(x) + i/2l$ is used at any point x in the well. If we make the hypothesis that the potential varies smoothly enough that a semiclassical approximation is valid, we obtain^{24–26}

$$M_w \approx \begin{bmatrix} \gamma^{-1} & 0 \\ 0 & \gamma \end{bmatrix}, \quad (2)$$

where

$$\gamma = \exp \left\{ i \int_0^w k_i(x) dx \right\}. \quad (3)$$

The transfer matrix M_{db} for the whole double-barrier structure is given by^{23–26}

$$M_{db} = M_1 M_w M_2 = \begin{bmatrix} 1/t_{db}^{(l)} & -r_{db}^{(r)}/t_{db}^{(l)} \\ r_{db}^{(l)}/t_{db}^{(l)} & [t_{db}^{(l)} - r_{db}^{(l)} r_{db}^{(r)}/t_{db}^{(l)}] \end{bmatrix}, \quad (4)$$

where $t_{db}^{(l)}$ and $r_{db}^{(l)}$ are the transmission and reflection coefficients, respectively, for an electron coming from the left, and $t_{db}^{(r)}$ and $r_{db}^{(r)}$ are the corresponding coefficients for an electron coming from the right electrode. Straightforward calculation yields²⁶

$$t_{db}^{(l)} = \frac{t_1^{(l)} t_2^{(l)} \gamma}{1 - c} \quad (5)$$

and

$$r_{db}^{(l)} = r_1^{(l)} \frac{1 - c/R_1}{1 - c}, \quad (6)$$

where

$$c = r_1^{(r)} r_2^{(l)} \gamma^2. \quad (7)$$

The expressions for $t_{db}^{(r)}$ and $r_{db}^{(r)}$ can be easily obtained from (5) and (6) by substituting the subscripts l with r , 1 with 2, and vice versa. An electron coming from the left has a

probability $T_{\text{db}}^{(l)} = |t_{\text{db}}^{(l)}|^2 k_{2r}/k_{1l}$ of being transmitted and a probability $R_{\text{db}}^{(l)} = |r_{\text{db}}^{(l)}|^2$ of being reflected; there is also a fraction $S_{\text{db}}^{(l)} = 1 - (T_{\text{db}}^{(l)} + R_{\text{db}}^{(l)})$ of electrons which have been absorbed (i.e., have undergone incoherent processes). In a completely analogous way we can define the corresponding probabilities $T_{\text{db}}^{(r)}$, $R_{\text{db}}^{(r)}$, and $S_{\text{db}}^{(r)}$ for an electron coming from the right. We also obtain that $T_{\text{db}}^{(l)} = T_{\text{db}}^{(r)}$ —hence we will often write simply T_{db} —while, in general, $R_{\text{db}}^{(l)} \neq R_{\text{db}}^{(r)}$.

III. DENSITY OF STATES IN THE CASE OF COHERENT TRANSPORT

In this section we will address the case of no incoherent process in the well, i.e., the mean-free path $l \rightarrow \infty$. In this case we have $R_{\text{db}}^{(l)} = R_{\text{db}}^{(r)} = R_{\text{db}} = 1 - T_{\text{db}}$ and the results of Ref. 1 can be straightforwardly applied.

We showed¹ that the density of states in a given system is equal to the sum of dwell times corresponding to each incoming channel divided by Planck's constant. In our case the region Ω of interest is (a, b) , and there are two incoming channels, the left and the right ones, so that the density of states $\rho_{\Omega}(E)$ in Ω , including both spin contributions, can be written as

$$\rho_{\Omega}(E) = \frac{1}{\pi\hbar} [\tau_D^{(l)}(E) + \tau_D^{(r)}(E)], \quad (8)$$

where $\tau_D^{(l)}$ and $\tau_D^{(r)}$ are the dwell times for an electron of energy E coming from the left and the right electrodes, respectively.

In order to obtain $\tau_D^{(l)}$ to substitute in (8), we can use the additivity of transmission and reflection times $\tau_T^{(l)}$ and $\tau_R^{(l)}$ obtained by using the Larmor clock and other well-known approaches.^{11–18} If we consider an electron coming from the left electrode, apply a uniform perturbative potential λ on the double barrier ($a < x < b$), and recalculate the total transmission and reflection coefficients as a function of λ , we can write

$$\tau_T^{(l)} \equiv \text{Re} \left\{ i\hbar \frac{\partial}{\partial \lambda} \ln t_{\text{db}}^{(l)} \right\} \bigg|_{\lambda=0}, \quad (9)$$

$$\tau_R^{(l)} \equiv \text{Re} \left\{ i\hbar \frac{\partial}{\partial \lambda} \ln r_{\text{db}}^{(l)} \right\} \bigg|_{\lambda=0}, \quad (10)$$

and, finally, obtain^{14–18} $\tau_D^{(l)} = \tau_T^{(l)} T_{\text{db}} + \tau_R^{(l)} R_{\text{db}}$. In the Introduction we mentioned the controversy on the tunneling time problem, and we are aware of the fact that there is no wide consensus in the scientific community on the “actual” significance of $\tau_T^{(l)}$ and $\tau_R^{(l)}$. Anyway, reassuring the reader that we do not want to forget about the long debate in this field, for convenience reasons we will refer to (9) and (10) as transmission and reflection times.

Substitution of (5) and (6) in (9) and (10), after straightforward but cumbersome calculations, yields

$$\tau_D^{(l)} = \tau_{T1}^{(l)} T_{\text{db}} + \tau_{R1}^{(l)} R_{\text{db}} + \tau_w T_{\text{db}} + \tau_{T2}^{(l)} T_{\text{db}} + \tau_{\text{rt}} T_1 \frac{|c|^2}{|1-c|^2}, \quad (11)$$

where $\tau_{T1}^{(l)}$, $\tau_{T2}^{(l)}$, and τ_w are the transmission times for barriers 1 and 2, and the well, respectively, defined as $\tau_T^{(l)}$ in (9) replacing $t_{\text{db}}^{(l)}$ with $t_1^{(l)}$, $t_2^{(l)}$, and γ , respectively; $\tau_{R1}^{(l)}$ is the reflection time for barrier 1, defined as $\tau_R^{(l)}$ in (10) with $r_1^{(l)}$ in the place of $r_{\text{db}}^{(l)}$. We call τ_{rt} *round trip time*; it is defined as

$$\tau_{\text{rt}} \equiv \text{Re} \left\{ \frac{i\hbar}{c} \frac{\partial c}{\partial \lambda} \right\} = \tau_{R1}^{(r)} + 2\tau_w + \tau_{R2}^{(l)}; \quad (12)$$

the last equality derives from (7) and explains the name given to τ_{rt} : it is actually the sum of the times corresponding to the steps needed for a round trip of the well: reflection from barrier 1, traversal of the well, reflection from barrier 2, and again traversal of the well. We can easily obtain $\tau_D^{(r)}$ by repeating all the passages from (4) to (11) commuting the subscripts l with r , and 1 with 2. If we substitute (11) and the corresponding result for $\tau_D^{(r)}$ into (8) we obtain

$$\rho_{\Omega}(E) = \frac{1}{\pi\hbar} \left[(\tau_{T1}^{(l)} T_{\text{db}} + \tau_{R1}^{(l)} R_{\text{db}}) + (\tau_{T2}^{(r)} T_{\text{db}} + \tau_{R2}^{(r)} R_{\text{db}}) + (\tau_{T2}^{(l)} + 2\tau_w + \tau_{T1}^{(r)}) T_{\text{db}} + \tau_{\text{rt}} \frac{|c|^2}{|1-c|^2} (T_1 + T_2) \right]; \quad (13)$$

$\rho_{\Omega}(E)$ includes all the states in the region ($a < x < b$). We are actually interested in the states in the well region and in the tail states penetrating both barriers on the well side, i.e., the states in the “effective” well region; therefore we drop from ρ_{Ω} the terms which take into account the states on the left side of barrier 1 and on the right side of barrier 2 [i.e., the first and the second terms of (13), respectively]. Moreover, the third term is easily shown to be much smaller (under the condition $T_1, T_2 \ll 1$) than the fourth one; therefore, the density of states ρ_w in the effective well region can be written as

$$\rho_w(E) = \frac{1}{\pi\hbar} \tau_{\text{rt}} \frac{|c|^2}{|1-c|^2} (T_1 + T_2). \quad (14)$$

From (7) and from the fact that $T_1, T_2 \ll 1$ we have $|c|^2(T_1 + T_2) \approx 1 - |c|^2$, so we get

$$\rho_w = \frac{1}{\pi\hbar} \tau_{\text{rt}} F(c), \quad (15)$$

where we have defined

$$F(c) \equiv \frac{1 - |c|^2}{|1 - c|^2}. \quad (16)$$

The density of states in the effective well region is therefore shown to be proportional to the round trip time times a factor $F(c)$, which will be shown in the next section to depend only upon transmission and reflection probabilities for the whole structure and for each barrier.

IV. DENSITY OF STATES IN THE PRESENCE OF INCOHERENT PROCESSES

A. Local density of states in the well

In this section incoherent processes are taken into account; therefore the formula (8) for the density of states is no

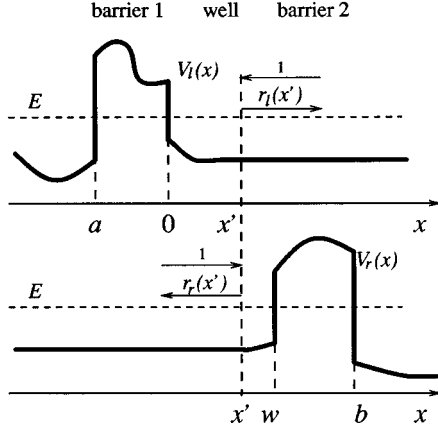


FIG. 2. The double-barrier structure is split into two regions at $x=x'$: $r_r(x')$ is the reflection coefficient for a plane wave of energy E incident on $V_r(x)$ from the left and $r_l(x')$ is the reflection coefficient for a plane wave of energy E incident on $V_l(x)$ from the right.

longer applicable. The total density of states ρ_w in the effective well region is obtained as the sum of the density of tail states $\rho_1^{(r)}(E)$ and $\rho_2^{(l)}(E)$ penetrating both barriers on the well sides (Sec. IV B) and the integral of the local density of states $\rho(x, E)$ in the well.

In this section, in particular, we obtain a formula for $\rho(x, E)$ which does not require the hypothesis of smooth potential in the well. We consider a point x' inside the well [$x' \in (0, w)$]. Let us split the x axis into two regions, and let us consider the potentials $V_l(x) \equiv V(x)$ for $x < x'$ and $V(x')$ otherwise, and $V_r(x) \equiv V(x)$ for $x > x'$ and $V(x')$ otherwise, as sketched in Fig. 2. Let us call $r_l(x')$ the reflection coefficient for a plane wave of energy E incident on $V_l(x)$ from the right, and $r_r(x')$ the reflection coefficient for a plane wave of energy E impinging on $V_r(x)$ from the left. The local density of states at a point x' can easily be written as¹

$$\rho(x', E) = \frac{1}{\pi\hbar} \sum_{n=1}^2 \frac{|\psi_n(x', E)|^2}{J_n(E)}, \quad (17)$$

where both spin contributions have been considered, the wave functions are not normalized, and $J_n(E)$ is the total current associated to state ψ_n entering the whole system. The sum is over all degenerate states corresponding to the same energy E , i.e., in our case, the ones associated to a particle coming from the left electrode ($n=1$) and a particle coming from the right electrode ($n=2$). The quantities to be put in (17) are derived in the Appendix. Substitution of (A1) and (A2) and the corresponding quantities for ψ_2 in (17) yields

$$\rho(x', E) = \frac{1}{\pi\hbar} \operatorname{Re} \left\{ \frac{(1 + r_r(x'))(1 + r_l(x'))}{1 - r_r(x')r_l(x')} \right\}. \quad (18)$$

An identical result has been obtained through different procedures and in simplified conditions by other authors.^{9,28}

B. Density of tail states penetrating both barriers on the well sides

For obtaining the density of tail states penetrating both barriers on the well sides we just have to use (17), provided that the sum is only over the states incident on the well side of the barriers. Let us consider the first barrier: the density of tail states $\rho_1^{(r)}$ is

$$\rho_1^{(r)}(E) = \frac{1}{\pi\hbar} \sum_{n=1}^2 \frac{\int_a^0 |\psi_n(x, E)|^2 dx}{J_n(E)}. \quad (19)$$

We can find for $\rho_1^{(r)}$ a more compact expression: in the Appendix we derived the currents $J_{1\text{inc}}^{(r)}(x, E)$ and $J_{2\text{inc}}^{(r)}(x, E)$ incident on $V_l(x)$, associated to the states ψ_1 and ψ_2 , respectively. Therefore, if we remember that the dwell time is defined as the ratio of the integral of the probability density over the considered region to the incident current, from (A3) and (A4) we can write

$$\begin{aligned} \rho_1^{(r)}(E) &= \frac{1}{\pi\hbar} \left[\frac{J_{1\text{inc}}^{(r)}(0, E)}{J_1(E)} + \frac{J_{2\text{inc}}^{(r)}(0, E)}{J_2(E)} \right] \tau_{D1}^{(r)} \\ &= \frac{1}{\pi\hbar} \tau_{D1}^{(r)} F[r_r(0)r_l(0)], \end{aligned} \quad (20)$$

where the function F has been already defined in (16).

For the second barrier, following the same procedure, we have

$$\rho_2^{(l)}(E) = \frac{1}{\pi\hbar} \tau_{D2}^{(l)} F[r_r(w)r_l(w)]. \quad (21)$$

C. Density of states in the effective well region

The density of states in the effective well region is, therefore, from (18), (20), and (21),

$$\rho_w(E) = \rho_1^{(r)}(E) + \rho_2^{(l)}(E) + \int_0^w \rho(x, E) dx. \quad (22)$$

We can write $\rho(x, E)$ in a different way, in order to derive a more compact formula for $\rho_w(E)$. Let the density matrix $\hat{g}(E)$ in the well be the incoherent superposition of states ψ_1 and ψ_2 with probabilities p_1 and p_2 , i.e.,

$$\langle x | \hat{g}(E) | x \rangle = p_1 |\psi_1(x)|^2 + p_2 |\psi_2(x)|^2. \quad (23)$$

Associated to $\hat{g}(E)$ there is the probability density current $J(E)$, whose expression is given by (A1) and the corresponding quantity for ψ_2 , that can be split into a left-going component $J_l(x, E) = p_1 J_{1\text{inc}}^{(l)}(x, E) + p_2 J_{2\text{inc}}^{(l)}(x, E)$ and a right-going component $J_r(x, E) = p_1 J_{1\text{inc}}^{(r)}(x, E) + p_2 J_{2\text{inc}}^{(r)}(x, E)$. Now, we can make the hypothesis that both J_l and J_r are much greater than the net current $J = J_l - J_r$. By imposing $J_r \approx J_l$ we can obtain J_r , J_l , and $\langle x | \hat{g}(E) | x \rangle$ as a function of p_1/p_2 . This result, substituted in (18), yields

$$\rho(x', E) = \frac{1}{\pi\hbar} \frac{\langle x | \hat{g}(E) | x \rangle}{J_l(x', E) + J_r(x', E)} F[r_l(x')r_r(x')]. \quad (24)$$

A great simplification of (22) can be obtained if we again make the semiclassical approximation in the well. In fact, in this case we have just to notice that $r_r(x')r_l(x')=c$ for all $x \in (0, w)$. Therefore we can write

$$\rho_w(E) = \frac{1}{\pi\hbar} \tau_{\text{rt}}^i F(c), \quad (25)$$

where we have defined

$$\tau_{\text{rt}}^i \equiv \tau_{D1}^{(r)} + \tau_{D2}^{(l)} + 2 \int_0^w \frac{\langle x' | \hat{g}(E) | x' \rangle}{J_l(x') + J_r(x')} dx'; \quad (26)$$

τ_{rt}^i can be interpreted as the round trip time of the well in the presence of inelastic processes. We wish to point out that (25) is formally analogous to (15) found in the case of coherent transport. It is also easy to verify that when $l \rightarrow \infty$, i.e., when the limit of coherent transport is approached, τ_{rt}^i tends to the value of τ_{rt} defined in (12).

The condition $T_1, T_2 \ll 1$ allows us to write, with very good approximation, the following expression for $F(c)$, where T_{db} , $R_{\text{db}}^{(r)}$, and $R_{\text{db}}^{(l)}$ are obtained from (5) and (6):

$$F(c) \approx \frac{1 - R_{\text{db}}^{(l)}}{T_1} + \frac{T_{\text{db}}}{T_2} \approx \frac{1 - R_{\text{db}}^{(r)}}{T_2} + \frac{T_{\text{db}}}{T_1}; \quad (27)$$

therefore (25) can be written as

$$\rho_w(E) \approx \frac{1}{\pi\hbar} \tau_{\text{rt}}^i \left[\frac{1 - R_{\text{db}}^{(l)}}{T_1} + \frac{T_{\text{db}}}{T_2} \right], \quad (28)$$

i.e., as a function of the round trip time and transmission and reflection probabilities for the total structure and for each barrier.

V. COMPARISON WITH BREIT-WIGNER FORMULAS

In this section we want to show that for a rate of incoherent processes low enough (i.e., a long enough mean-free path), the formula for the density of states derived above reduces to the one obtained by means of Breit-Wigner formulas.

Let us expand c given by (7) to first order around the resonant energy E_R (which is the energy at which c is real and positive):

$$c(E) \approx c(E_R) \left[1 - i \frac{\tau_{\text{rt}}^i(E_R)}{\hbar} (E - E_R) \right], \quad (29)$$

where we have used the definition (12) of τ_{rt} and the fact that $\arg\{i\hbar \partial \ln c / \partial E\} \approx 0$. If w/l is small enough we can write

$$\begin{aligned} c(E_R) &= [R_1(E_R)R_2(E_R)]^{1/2} e^{-w/l} \\ &\approx 1 - \frac{1}{2}T_1(E_R) - \frac{1}{2}T_2(E_R) - \frac{w}{l}. \end{aligned} \quad (30)$$

Substitution of (29) and (30) into (5) and (6) yields

$$T_{\text{db}} \approx \frac{\Gamma_1 \Gamma_2}{(E - E_R)^2 + (\Gamma/2)^2} \quad (31)$$

and

$$1 - R_{\text{db}}^{(l)} \approx \frac{\Gamma_1(\Gamma_2 + \Gamma_i)}{(E - E_R)^2 + (\Gamma/2)^2}, \quad (32)$$

where $\Gamma_1 = \hbar T_1(E_R)/\tau_{\text{rt}}^i(E_R)$, $\Gamma_2 = \hbar T_2(E_R)/\tau_{\text{rt}}^i(E_R)$, $\Gamma_i = \hbar 2w/[\tau_{\text{rt}}^i(E_R)l]$, and $\Gamma = \Gamma_1 + \Gamma_2 + \Gamma_i$.

Equations (31) and (32) are the Breit-Wigner formulas,^{2,4,29} and Γ_1 , Γ_2 , and Γ_i are the partial resonance widths for each process allowing escape from the resonant state, in particular, tunneling through barriers 1 and 2, and incoherent processes, respectively. Partial resonant widths are characteristic quantities of the Breit-Wigner formalism, and are given by the ratio between \hbar and the characteristic time of the process we are considering. In the case of escape through one of the barriers, the characteristic time is intuitively given by the ratio of the round trip time and the tunneling probability of the barrier. In the case of inelastic scattering the time is τ_{rt} times the ratio between the mean-free path l and the length corresponding to a round trip of the well ($2w$).

From (28) and (31) and (32), we straightforwardly have

$$\rho_w(E) \approx \frac{1}{\pi} \frac{\Gamma}{(E - E_R)^2 + (\Gamma/2)^2}, \quad (33)$$

i.e., the result usually obtained from Breit-Wigner formulas.^{3,4} We wish to point out that this formula holds true if the development of c to first order of $E - E_R$ and to first order in w/l is a good approximation. In other words, Breit-Wigner formulas can be used if each partial width is much smaller than both the resonant energy E_R and the difference between the height of the barriers and E_R . In our case these conditions are true for Γ_1 and Γ_2 and hold true for Γ_i if l/w is high enough. Otherwise, the expression given by (25), which has a wider range of applicability, has to be used.

VI. SUMMARY

In this paper we have studied the density of states in a double-barrier structure. We have proposed a simple model which is able to account for inelastic processes occurring in the quantum well by means of a single phenomenological parameter l , the mean-free path.

We have obtained a very compact formula which relates the density of states in the effective well region to the round trip time of the quantum well and to the tunneling probabilities for the single barriers and for the whole structure. The formula is valid both in the case of completely coherent transport and in the case when dissipative processes in the well are predominant.

This formula will be shown to be fundamental in unifying two widely known descriptions of transport in double-barrier structures: that of resonant tunneling and that of sequential tunneling.¹⁰

We believe that the role of the density of states—a characteristic quantity of a system in equilibrium—in the steady state transport and in the characteristic times of the motion of electrons in a mesoscopic system deserves a deeper investigation.

ACKNOWLEDGMENTS

The present work has been supported by the Ministry for the University and Scientific and Technological Research of Italy, and by the Italian National Research Council (CNR).

APPENDIX

Let us consider a point $x=x'$ in the well and the state ψ_1 of energy E corresponding to a particle coming from the left of x' . We can describe ψ_1 as a plane wave of amplitude 1 undergoing multiple reflections on $V_r(x)$ for $x>x'$ and $V_l(x)$ for $x<x'$ (see Figs. 1 and 2), so that we have

$$\psi_1(x') = 1 + r_r(x') + r_r(x')r_l(x') + \dots = \frac{1 + r_r(x')}{1 - r_r(x')r_l(x')}. \quad (\text{A1})$$

Now, $[1 - |r_l(x')|^2]$ is the probability that a particle impinging on $V_l(x)$ is not reflected back (i.e., is either transmitted or “absorbed” on the left of x'). For time reversal symmetry, it is also the probability that an electron coming from the left of x' appears at $x=x'$: if 1 is the amplitude of ψ_1 before taking into account multiple reflections, the total current entering the system has to be

$$J_1 = \frac{v(x')}{1 - |r_l(x')|^2}, \quad (\text{A2})$$

where $v(x) = \hbar k(x)/m$. It is worth noticing that the dependence of J_1 on x' is due only to the fact that ψ_1 is not normalized. We can also associate to ψ_1 and x' a probability current density which can be split into a left-going component $J_{\text{inc}}^{(l)}$ [incident on $V_l(x)$] and a right-going component $J_{\text{inc}}^{(r)}$ [incident on $V_r(x)$],

$$J_{\text{inc}}^{(l)}(x') = \frac{|r_r(x')|^2 v(x')}{|1 - r_l(x')r_r(x')|^2} \quad (\text{A3})$$

and

$$J_{\text{inc}}^{(r)}(x') = \frac{v(x')}{|1 - r_l(x')r_r(x')|^2}. \quad (\text{A4})$$

The corresponding quantities for the state ψ_2 , associated to a particle coming from the right of $x=x'$, can be obtained by substitution of 1 with 2, r with l , and vice versa.

*Fax number: ++39-50-568522; electronic address: ianna@pimac2.iet.unipi.it

¹G. Iannaccone, Phys. Rev. B **51**, 4727 (1995).

²L. D. Landau and E. M. Lifshitz, *Quantum Mechanics (Non-Relativistic Theory)* (Pergamon Press, Oxford, 1977), p. 603.

³T. Weil and B. Vinter, Appl. Phys. Lett. **50**, 1281 (1987).

⁴M. Büttiker, IBM J. Res. Dev. **32**, 63 (1988).

⁵A. D. Stone and P. A. Lee, Phys. Rev. Lett. **54**, 1196 (1985).

⁶M. Jonson and A. Grincwajg, Appl. Phys. Lett. **51**, 1729 (1987).

⁷N. W. Ashcroft and N. D. Mermin, *Solid State Physics* (Saunders College, Philadelphia, 1976), pp. 9, 52, 244–246. Relevant characteristic lengths of electron motion are discussed by C. W. J. Beenakker and H. van Houten, in *Solid State Physics*, edited by H. Ehrenreich and D. Turnbull (Academic Press, Boston, 1991), Vol. 44, pp. 7, 19–23, 36–49.

⁸Equations (A4)–(A12) of Ref. 4 imply that transmission and reflection probabilities do not depend upon energy, i.e., that electrode chemical potentials are close enough that electrons contributing to the net current have energies in a very narrow energy range. Otherwise, the incoherent transmission probability in (A12) of Ref. 4 is still valid, provided that we do not include energy relaxation in the extra reservoir and impose on the extra branch that all current contributions at any energy be zero, and not only the net current flow.

⁹A. Knäbchen, Phys. Rev. B **45**, 8542 (1992).

¹⁰G. Iannaccone and B. Pellegrini, Phys. Rev. B **52**, 17 406 (1995).

¹¹A. I. Baz', Yad. Fiz. **5**, 229 (1966) [Sov. J. Nucl. Phys. **5**, 161 (1967)].

¹²D. Sokolovski and L. M. Baskin, Phys. Rev. A **36**, 4604 (1987).

¹³M. Büttiker, Phys. Rev. B **27**, 6178 (1983).

¹⁴C. R. Leavens and G. C. Aers, Phys. Rev. B **40**, 5387 (1989).

¹⁵E. H. Hauge and J. A. Støvneng, Rev. Mod. Phys. **61**, 197 (1989).

¹⁶C. R. Leavens, Solid State Commun. **74**, 923 (1990).

¹⁷G. Iannaccone and B. Pellegrini, Phys. Rev. B **49**, 16 548 (1994).

¹⁸G. Iannaccone and B. Pellegrini, Phys. Rev. B **50**, 14 662 (1994).

¹⁹R. Landauer and Th. Martin, Rev. Mod. Phys. **66** 217 (1994).

²⁰J. R. Barker, S. Brouard, V. Gasparian, G. Iannaccone, A. P. Jauho, C. R. Leavens, J. G. Muga, R. Sala, and D. Sokolovski, Phantoms Newsletter **7**, 5 (1994).

²¹J. G. Muga, S. Brouard, and R. Sala, J. Phys. Condens. Matter **4**, L579 (1992).

²²These points are no longer controversial if one adopts Bohm's interpretation of quantum mechanics; see C. R. Leavens and G. C. Aers, in *Scanning Tunneling Microscopy III*, edited by R. Wiesendanger and H.-J. Güntherodt, Springer Series in Surface Sciences Vol. 29 (Springer-Verlag, Berlin, 1993), p. 105.

²³P. Erdős and R. C. Herndon, Adv. Phys. **31**, 64 (1983).

²⁴B. Riccò and M. Ya. Azbel, Phys. Rev. B **29**, 1970 (1984).

²⁵D. K. Ferry, in *Physics of Quantum Electron Devices*, edited by F. Capasso (Springer-Verlag, Berlin, 1990), p. 77.

²⁶H. C. Liu and T. C. L. G. Sollner, Semicond. Semimet. **41**, 359 (1994).

²⁷Y. Ando and T. Itoh, J. Appl. Phys. **61**, 1497 (1987).

²⁸A. Modinos, G. C. Aers, and B. V. Paranjape, Phys. Rev. B **19**, 3996 (1979).

²⁹G. García Calderón and A. Rubio, Solid State Commun. **71**, 237 (1989).