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Semiclassical description of resonant tunneling

E.B. Bogomolny[a] and D.C. Rouben

Laboratoire de Physique Théorique et Modèles Statistiques, Bâtiment 100, 91405 Orsay Cedex, France

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Abstract. We derive a semiclassical formula for the tunneling current of electrons trapped in a potential well which can tunnel into and across a wide quantum well. The tunneling current is measured at the second interface of this well and our calculations idealized an experimental situation where a strong magnetic field tilted with respect to an electric field was used. It is shown that the contribution to the tunneling current, due to trajectories which begin at the first interface and end on the second, is dominant for special periodic orbits which hit both walls of the quantum well and are perpendicular to the first wall. The resulting formula, which is a semiclassical expression for the total tunneling current, differs in a few important aspects from the Gutzwiller trace formula for the density of states. The Miller-type modification of the obtained semiclassical formula for stable orbits is also discussed.

PACS. 03.65.Sq Semiclassical theories and applications – 05.45.MT Semiclassical chaos ("quantum chaos")

1 Introduction

The statistical properties of the energy level spectrum of a classically chaotic system is now well understood, largely through the theoretical work of Balian and Bloch [1], Gutzwiller [2] and Berry [3] as well as others [4]. In particular these authors were searching for a correspondence between the classical mechanics of a dynamical system and the quantum mechanical properties of the dynamical system. From these investigations, several important theoretical and experimental developments were made to explain the quantum-classical correspondence. A first and central result of this work, the trace formula, relates long-range fluctuations in the density of quantized levels to underlying classical periodic orbits (PO). Each PO of the classical dynamical system with period T_p generates regular maxima in the level density separated by an energy $\Delta E_p = \hbar/T_p$. Theoretical studies have also tried to find a connection between wavefunctions and eigenstates of the Hamiltonian with the dynamics of classical systems exhibiting chaotic motion. This investigation has given rise to the discussion of wavefunction scarring by a periodic orbit or sets of periodic orbits (see *e.g.* [5,6]). In the case where the classical motion is regular in the whole phase space (*i.e.* when the system is said to be integrable) a clear and complete correspondence between the quantum and classical pictures of the system can be made in the semiclassical limit $\hbar \to 0$. In particular, one can generate from the classical motion on tori, eigenvalues and eigenfunctions of the Hamiltonian *via* semiclassical $\hbar \to 0$ arguments. These arguments are, of course, not applicable to classical systems exhibiting chaotic dynamics and for which quantization rules are still a subject of research.

The influence of classical chaotic motion on the quantum mechanical system has also been investigated experimentally. For example, periodic modulations in the magnetoabsorption spectra of highly-excited hydrogenic atoms are correlated with fluctuations in the density of states due to closed orbits at energies close to the ionization potential [7,8]. Still more recently similar observations were made from the oscillatory structure found in the low-field magnetoresistance spectrum of anti-dot superlattices, the cause of which was attributed to fluctuations in the density of states from unstable periodic orbits encircling a small number of anti-dots [9].

In this paper we investigate a particular system to which much experimental work has been devoted in recent years [10,11]. The double well potential consisting of GaAs/(AlGa)As resonant tunneling diodes (RTDs) containing a wide quantum well (QW) has been used to explore a relationship between the classical and quantum pictures of electron dynamics. In the presence of a large uniform magnetic field tilted with respect to the z-axis by an angle θ and a uniform electric field parallel to the z-axis (see Fig. 1), the system exhibits chaotic motion for certain initial conditions in phase space [10–15]. Also it was found that the chaotic component in phase space increases as θ increases above 0. However, unstable periodic orbits in the chaotic sea were also found and were shown to have a profound effect on the QW energy spectrum as well as the peaks in the resonant tunneling spectrum of magnetotunneling spectroscopy. The latter, in particular, established a link between the current-voltage characteristics of the RTDs and the underlying classical motion in the QW.

[a] e-mail: bogomol@ipno.in2p3.fr

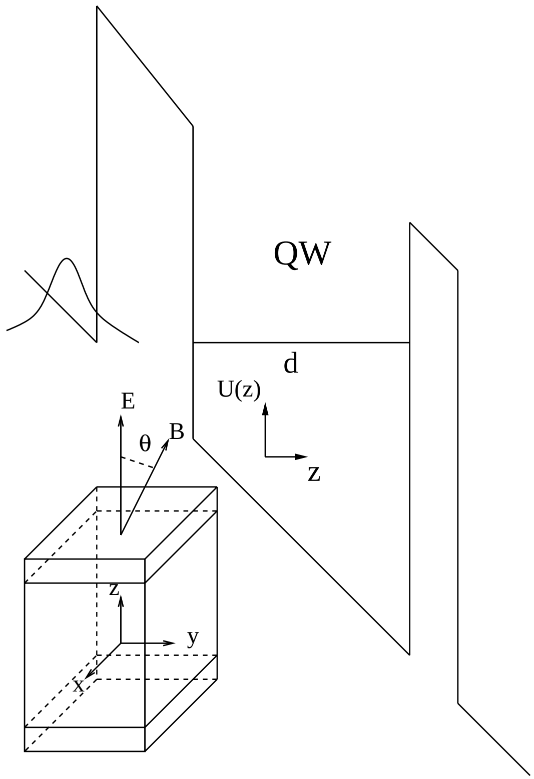

Fig. 1. Arrangement of the quantum well.

The main purpose of this paper is to obtain a quantitative description of this link. In previous papers [10–15], the Gutzwiller trace formula for the density of states was used to specify the relationship between classical periodic orbits and the tunneling current. But it is clear that the Gutzwiller formula cannot be immediately applied to tunneling phenomena since the density of states is expressed as a sum over all periodic orbits and it is physically evident that the resonant tunneling formula has to be connected only with orbits which start on the LH wall and end on the RH one (*i.e.* orbits which hit the RH wall at least once before evacuating). The contribution from other orbits should be small in the semiclassical regime.

We shall derive a semiclassical formula for the resonant tunneling current and show that the major contribution to the tunneling current will be from special periodic trajectories which hit the two walls and are perpendicular to the first wall. The main difference of the obtained expression for the tunneling current and the usual Gutzwiller trace formula is that the prefactor is inversely proportional to the square root of m_{21} monodromy matrix element for the former and to $(m_{11} + m_{22} - 2)$ element for the later. A short account of our results has been published in [16].

The problem of resonant tunneling differs from that of the density of states by the condition that the electron has a well defined initial state which can tunnel into the QW and which, after some motion therein, can escape from the device. Assuming that the tunneling probabilities are small (and ignoring the possibility of tunneling from the QW back to the emitter) one naturally comes to a sequential theory of tunneling [17] according to which one has to compute independently four main ingredients: (i) the initial state in the first well, (ii) the probability of tunneling through the first barrier, (iii) the motion inside the QW, (iv) the probability of tunneling through the second barrier.

The plan of the paper is the following. In Section 2 a general formulation of the problem is presented. In Section 3 an approximate wavefunction of the initial state localized in the emitter well is discussed. Section 4 is devoted to a description of a simple but clear picture of tunneling through potential barriers. In Section 5 we discuss the matching of the boundary value of the wave function with the Green function inside the QW. Then using the semiclassical expression for the Green function we derive in Section 6 the semiclassical formula for the tunneling current. The resulting expression is based on the assumption that pure semiclassical approximation can be applied for all trajectories.

In real experiments the semiclassical condition is sometimes violated for special trajectories at a particular value of external field and dimension of experimental devices. Therefore, corrections to the strict semiclassical formula are of importance. In Section 7 we discuss a simple modification which should be valid for regions of phase space where the classical dynamics is close to being integrable. In Section 8 the semiclassical approximation of a simplified model of resonant tunneling proposed in references [14,15] is derived and in Section 9 we discuss the Miller-type modification of semiclassical formulae which generalize the torus quantization of reference [15]. Two appendices are added to clarify certain technical points.

2 Formulation of the problem

The classical Hamiltonian for motion of an electron inside the system, in the presence of an electric field along the z-axis and a magnetic field tilted by an angle θ in the (y, z)-plane, can be written as follows:

$$H = \frac{(p_x - B_0 y \cos\theta + B_0 z \sin\theta)^2}{2m} + \frac{p_y^2}{2m} + \frac{p_z^2}{2m} - \varepsilon z + V(z), \quad (1)$$

where $V(z)$ is a step-wise potential modeling allowed-forbidden layers along the z-axis. The schematic view of effective potential $U(z) = -\varepsilon z + V(z)$ is presented in Figure 1.

In order to write the Hamiltonian in the above form we have used atomic units in which the magnetic field $B = B_0\ 2.35 \times 10^5$ T, the electric field $F = \varepsilon\ 5.14 \times 10^{11}$ V/m, the distance $R = r\ 0.53$ Å and $m = 0.067 m_{\mathrm{e}}$ is the band edge mass of an electron in GaAs.

In a typical experimental situation [10], $B = 11.4$ T and F is in the vicinity of 2.1×10^6 V/m which in atomic units corresponds to $B_0 = 4.85 \times 10^{-5}$ and $\varepsilon = 4.1 \times 10^{-6}$. The important parameter here is the length for which the influence of the electric field is of the same order as that of the magnetic field [11]: $l_0 = mF/eB^2$. For values above $l_0 \approx 60$ Å the magnetic field has as large an effect on the dynamics as the electric field. On the other hand, for smaller distances the electric field dominates and the effect of the magnetic field can be treated as a perturbation. In one experiment [10] the width of the QW was 1200 Å and both barriers have the width 56 Å. In [11] the LH barrier had the width 57 Å, the RH barrier 37 Å and the data was presented for QW of different thicknesses: 400, 600, 850, and 1200 Å. The scaling properties of this Hamiltonian have been discussed in [13].

Motion in the direction x is not free although clearly $\dot{p}_x = 0$. The dependence $x(t)$ can be obtained from integration of the equation

$$\dot{x} = \frac{1}{m}(p_x - B_0 y \cos\theta + B_0 z \sin\theta). \quad (2)$$

Since p_x is a constant of the motion the Hamiltonian in equation (1) is effectively two-dimensional and it follows that p_x can be removed by the shift: $y = \tilde{y} + p_x/B_0 \cos\theta$. This change leads to the 2d Hamiltonian:

$$H_2(\tilde{y}, z) = \frac{p_{\tilde{y}}^2}{2m} + \frac{p_z^2}{2m} + \frac{B_0^2}{2m}(\tilde{y}\cos\theta - z\sin\theta)^2 - \varepsilon z + V(z). \quad (3)$$

After the canonical change of variables

$$y' = \tilde{y}\cos\theta - z\sin\theta, \quad z' = \tilde{y}\sin\theta + z\cos\theta$$

this Hamiltonian is transformed to

$$H_2'(y', z') = \frac{p_{y'}^2}{2m} + \frac{B_0^2}{2m}y'^2 + \frac{p_{z'}^2}{2m} - \varepsilon(z'\cos\theta - y'\sin\theta) + V(z). \quad (4)$$

Notice that the previous form is composed of two uncoupled modes, the energy in each of which does not change as a function of time. It follows that the classical motion is integrable within the QW and that its numerical computation, using the Hamiltonian in equation (4), is easy in between collisions. For this reason we will work with this Hamiltonian and integrate the equations of motion in these variables (we convert back to the physical y and z coordinates using the formulas above).

It is the collisions with the walls (described by $V(z)$) which mix energy in the two modes and hence destroy the integrable nature of the problem. At $\theta = 0$ no such mixing occurs and the system is integrable, motion in phase space is on tori and WKB quantization can be applied to extract, semiclassically, all the quantum mechanical information desired. For $\theta > 0$ the motion is no longer integrable and the chaotic component of phase space in general increases as θ increases. Or if we increase B_0 at fixed θ, regular regions in phase space are destroyed and become chaotic (see the evolution in Fig. 2). It is in the chaotic regime that we will pursue an analysis and the tunneling current formula will be specific to the contribution from isolated unstable orbits submerged in a chaotic sea. For stable and almost stable orbits special approximations will be discussed later.

The quantum Hamiltonian has the same form as its classical analogue but p_y and p_z are considered as operators. The energy levels and wavefunctions of the problem can, in principle, be computed from a numerical solution of the Schrödinger equation. One of the difficulties encountered when tackling the problem of resonant tunneling is the form of the wavefunction in the emitter well. All the information of the electron, before tunneling has occurred, will be contained here. What to do with this wavefunction from the point of view of tunneling into the QW and a connection with motion therein are the problems that come after. We shall use a form for the initial state that facilitates subsequent treatment. This approach, outlined in the following sections, gives a good first approximation but at the same time its accuracy is limited by the simplicity of the initial state and the treatment of tunneling into the QW that follows this approximation. Nevertheless, because our main purpose is to derive a semiclassical trace formula for tunneling into the quantum well without a detailed account of the form of the initial state, we will use an oversimplified form for the initial state based on a perturbation theory expansion over the diamagnetic term (see *e.g.* [18]).

3 The initial state

The applied electric field puts the system under bias and accumulates charge in the emitter well. A bound (or quasi-bound) state at the emitter-QW interface at liquid-helium temperatures gives rise to a degenerate two-dimensional electron gas which is the initial state for electrons which tunnel into the QW. The formation of the emitter state depends on the exact shape of the confining potential and the mutual interaction between electrons and its correct description is a rather complicated problem. We will bypass these difficulties and treat the problem as described above.

The energy corresponding to the Hamiltonian (3), to first order, is given by $E = \langle\psi|\hat{H}|\psi\rangle$ where ψ is a zero order wavefunction which we will write in the following form:

$$\psi(y, z) = \psi(y)\chi(z). \quad (5)$$

$\chi(z)$ is a 1d wavefunction for motion in the z direction

$$\left(\frac{\hat{p}_z^2}{2m} + U(z)\right)\chi(z) = E_{(z)}\chi(z), \quad (6)$$

and $U(z)$ is a linear-wise effective potential along the z-direction.

The in-plane wavefunction $\psi_n(y)$ is given by the Landau level eigenfunction for motion in the magnetic field:

$$\left(\frac{1}{m}(B_{\|}y + B_{\perp}\langle z\rangle)^2 + \frac{\hat{p}_y^2}{2m}\right)\psi(y) = E_{(x,y)}\psi(y), \quad (7)$$

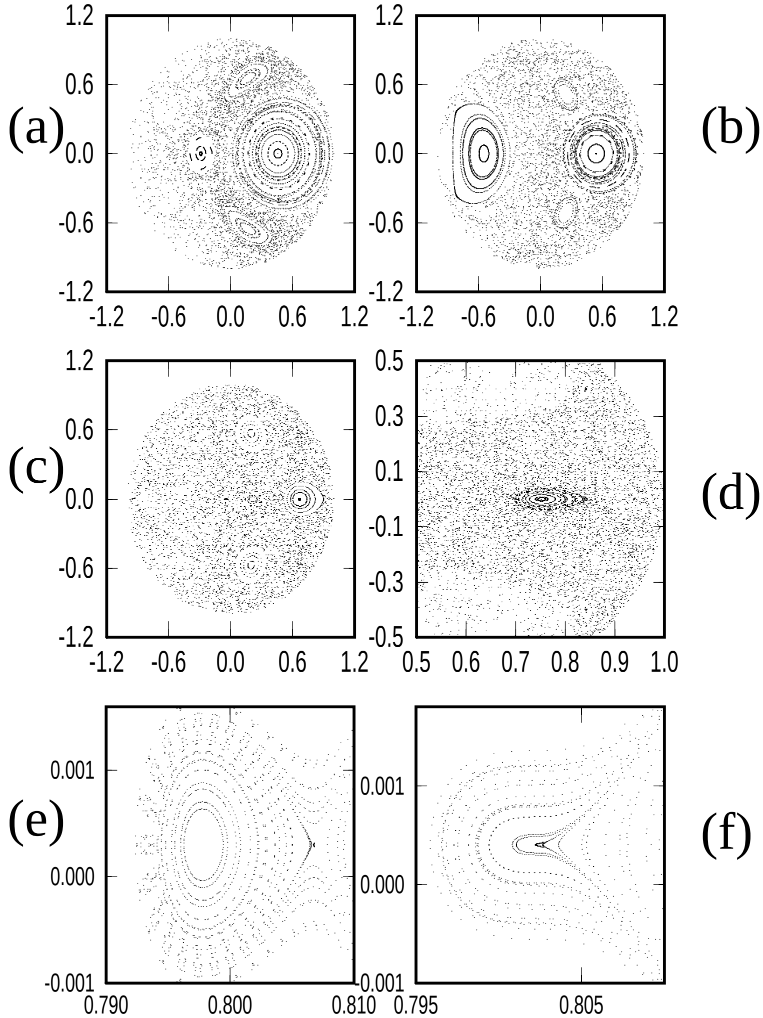

Fig. 2. Poincaré surfaces of section at $\theta = 11°$, $\varepsilon = 8 \times 10^{-6}$ and $z = 0$ for different magnetic field. We plot $\dot{y}/\dot{y}_\circ$ *versus* $y/y_\circ$ with $y_\circ = \sqrt{2mE/\beta}$ and $\dot{y}_\circ = \sqrt{2E/m}$. The large stable region on the right in (a) corresponds to a one bounce periodic orbit, the one on the left to a four bounce periodic orbit. As the magnetic field increases, this stable region shifts to the right on the surface of section, (b), (c), (d) and finally disappears in a tangent bifurcation, (e), (f) at $B_\circ \approx 3.47 \times 10^{-5}$.

where $B_\parallel = B_0 \cos\theta$ and $B_\perp = B_0 \sin\theta$ (parallel and perpendicular with respect to the electric field). Note that there is a shift due to the diamagnetic term in the perturbation expansion and the corresponding energy becomes the sum of three terms:

$$E = E_{(z)} + E_{(\mathrm{diam})} + E_{(x,y)}. \tag{8}$$

The first term is an unperturbed sub-band energy in the first well for the wavefunction $\chi(z)$, the second is the diamagnetic shift

$$E_{(\mathrm{diam})} = \frac{B_\perp^2}{2m}(\langle z^2\rangle - \langle z\rangle^2),$$

where $\langle \ldots \rangle = \int \chi(z) \ldots \chi(z) \mathrm{d}z$ is a mean value over the function $\chi(z)$, and the third term is the energy of the Landau level for the in-plane (x, y) problem

$$E_{(x,y)} = (n + 1/2)B_\parallel/m.$$

At sufficiently large magnetic field and at low temperatures the system will occupy only the lowest lying state with $n = 0$. The corresponding in-plane eigenfunction (with $p_x = 0$) is

$$\psi_0(y) = \left(\frac{B_\parallel}{\pi}\right)^{1/4} \exp\left(-\frac{1}{2}B_\parallel(y - \tilde{y})^2\right), \tag{9}$$

where $\tilde{y} = \langle z\rangle \tan\theta$ is a shift due to the diamagnetic term in the perturbation expansion.

The three terms in (8) have the following values:

$$\begin{aligned} E_{(z)} &= \alpha(\varepsilon^2/m)^{1/3}, \\ E_{(\mathrm{diam})} &= \beta B_\perp^2/(m)^{5/3}\varepsilon^{2/3}, \\ E_{(x,y)} &= \gamma B_\parallel/m, \end{aligned} \tag{10}$$

where α, β, γ are numerical factors on the order of unity ($\gamma = 1/2$).

For simplicity we shall use a variational anzats for the normalized wavefunction describing motion along the z-axis (see [18])

$$\chi(z) = 2a^{-3/2} z \exp(z/a), \quad -\infty \le z \le 0 \tag{11}$$

although the exact solution in terms of an Airy function is, of course, possible. We define the parameter a from the condition that it minimizes the energy functional

$$E_{(z)} = \int \chi \left(-\frac{1}{2m} \frac{\mathrm{d}^2}{\mathrm{d}z^2} + \varepsilon z \right) \chi \mathrm{d}z. \tag{12}$$

From this, one gets $a = (2/3)^{1/3}(m\varepsilon)^{-1/3}$ which gives $\beta = 3^{1/3} 2^{-7/3} \approx 0.3$ and $\alpha = (3/2)^{5/3} \approx 1.97$. (The exact solution of the Schrödinger equation with the linear potential, in terms of the Airy function under the assumption that the height of the barrier is very big gives for the lowest level $\alpha = 1.86$). For experimental values of the fields all three terms (putting $B_\parallel \approx B_\perp \approx B_0$) are approximately of the same order and the perturbation theory should be taken with more care. Still we shall use this approach as it permits us to have a clear initial picture of the problem at hand without adding further complications.

4 Tunneling

Knowing the form of the wave function in the first well one can compute the probability of tunneling through the first barrier. An important consequence of our treatment of the initial state wavefunction (6) is the fact that one has to consider only one dimensional tunneling in the z direction. The in-plane part of the whole wave function $\psi(x, y)$ remains the same throughout the tunneling process.

Let us evoke a few well-known and useful relationships for quasi-bound states important also to our analysis (see *e.g.* [19]). The conservation of the probability current

$$J_\mu = -\frac{\mathrm{i}}{2m}(\bar{\psi}\partial_\mu \psi - \partial_\mu \bar{\psi}\psi)$$

gives

$$\frac{\partial}{\partial t}|\psi(x,t)|^2 = -\partial_\mu J_\mu. \tag{13}$$

For a quasi-bound state $\psi(x,t) = \psi(x)\exp(-\mathrm{i}Et)$ the energy E must have an imaginary part Γ naturally associated with the possibility of tunneling

$$E = E_0 - \frac{\mathrm{i}}{2}\Gamma. \tag{14}$$

Integrating equation (13) over a large volume V surrounded by a surface B one gets

$$\Gamma = \frac{1}{\int_V |\psi|^2 \mathrm{d}v} \int_{\mathrm{B}} \mathbf{J} \mathrm{d}\boldsymbol{\sigma}. \tag{15}$$

Assuming that the tunneling probability is small, ψ is large only inside the initial well and the integral in the denominator can be taken just over the first well. Therefore to compute Γ it is necessary to know the current in the region where there is no possibility of returning back (or it is very small).

The calculations are particularly simple in the semiclassical approximation for one dimensional models. In one dimension the scattering on a barrier is characterized by the reflection (r) and transmission (t) coefficients which obey the relationship

$$|r|^2 + |t|^2 = 1. \tag{16}$$

The wave function before the barrier can be written as the sum of incoming and outcoming waves

$$\psi(x) = \psi_+(x) + r\psi_-(x), \tag{17}$$

and after the barrier it has to be described only by an outcoming wave

$$\psi(x) = t\psi_+(x) \tag{18}$$

where $\psi_\pm(x)$ are the standard semiclassical functions

$$\psi_\pm(x) = \frac{1}{\sqrt{k(x)}} \exp\left(\pm \mathrm{i} \int^x k(x')\mathrm{d}x' \right), \tag{19}$$

and $k(x) = \sqrt{2m(E - U(x))}$.

For a step-wise barrier

$$t = 2\mathrm{i}\sqrt{\sin 2\Phi_1 \sin 2\Phi_2}\, \mathrm{e}^{-\Delta} \mathrm{e}^{-\mathrm{i}(\Phi_1 + \Phi_2)} \times \frac{1}{1 - \mathrm{e}^{-2\Delta}\mathrm{e}^{-2\mathrm{i}(\Phi_1+\Phi_2)}}, \tag{20}$$

$$r = \mathrm{e}^{-2\mathrm{i}\Phi_1} \frac{1 - \mathrm{e}^{-2\Delta}\mathrm{e}^{2\mathrm{i}(\Phi_1 - \Phi_2)}}{1 - \mathrm{e}^{-2\Delta}\mathrm{e}^{-2\mathrm{i}(\Phi_1+\Phi_2)}}, \tag{21}$$

where

$$\tan \Phi_i = p(x_i)/k(x_i),$$
$$p(x) = \sqrt{2m(U_2(x) - E)},$$
$$\Delta = \int_{x_1}^{x_2} p(x)\mathrm{d}x,$$

and x_1 (x_2) correspond to the left (right) coordinate of the barrier.

When Δ is large

$$t = 2\mathrm{i}\sqrt{\sin 2\Phi_1 \sin 2\Phi_2}\, \mathrm{e}^{-\Delta}\mathrm{e}^{-\mathrm{i}(\Phi_1+\Phi_2)} \tag{22}$$

$$r = \mathrm{e}^{-2\mathrm{i}\Phi_1}\mathrm{e}^{-u} \tag{23}$$

and $u = 2\mathrm{i}\sin 2\Phi_1 \mathrm{e}^{-2\mathrm{i}\Phi_2}\mathrm{e}^{-2\Delta}$. Note that 2Φ plays the role of the additional phase shift for reflection on a wall of finite height.

Computation of the imaginary part of the quasi-bound state energy follows from knowledge of the transmission coefficient. In the semiclassical approximation in the first well $|\psi|^2 = 2/k(x)$ and one gets the standard formula

$$\Gamma = \frac{1}{T}|t|^2, \tag{24}$$

where

$$T = 2m \int \frac{\mathrm{d}x}{k(x)}$$

is the period of the classical motion in the first well. These formulas indicate that each time a particle, trapped in the emitter well, hits the barrier it has the probability of tunneling equal to the square of the tunneling coefficient and a probability of tunneling per unit time equal to the probability multiplied by the number of collisions per unit time, $1/T$. For lowest states the semiclassical approximation is not accurate and the prefactor in this formula should be modified.

Ignoring the tunneling, let $\psi_0(x)$ be a wave function inside the first well normalized by the usual condition $\int |\psi_0|^2 \mathrm{d}x = 1$. Then according to (18) the wave function just after the barrier is

$$\chi_1(z) = \frac{C}{\sqrt{k(z)}} \exp\left(\mathrm{i} \int_{x_2}^{z} k(z')\mathrm{d}z'\right), \tag{25}$$

where the modulus of the prefactor is determined by the imaginary part of the quasi-bound state

$$|C|^2 = m\Gamma_1. \tag{26}$$

We put here a subscript 1 to stress that this quantity has been computed for the first well.

5 Semiclassical matching

The next step is to compute the corresponding wavefunction in the interior of the QW and in particular on the second barrier wall at $z = d$. Call this wavefunction $\psi_2(y, z)$ and the tunneled wavefunction, in the vicinity of the emitter-QW interface, $z = 0$, $\psi_1(y, z)$. As discussed above, the initial state wavefunction was put in the separable form

$$\psi_1(y, z) = \chi_1(z)\psi_0(y), \tag{27}$$

where $\chi_1(z)$ is given by (25) and $\psi_0(y)$ by (9) but the following considerations are quite general and can be applied for many similar problems.

Because the QW is assumed to be wide we will calculate transmission probabilities between two points within the QW semiclassically and consider $\psi_1(y, z)$ to be a boundary value wavefunction, in the vicinity of $z = 0$, for the (unknown) function $\psi(y, z)$.

An explicit form of this function can be obtained from the usual boundary representation of wavefunctions as follows.

Let us consider the equations:

$$(E - \hat{H}^\dagger(\mathbf{x}))\psi(\mathbf{x}) = 0 \tag{28}$$

and

$$(E - \hat{H}(\mathbf{x}))G(\mathbf{x}', \mathbf{x}, E) = \delta(\mathbf{x}' - \mathbf{x}), \tag{29}$$

where $G(\mathbf{x}', \mathbf{x}, E)$ is a (retarded) Green function in the energy representation for motion from point $\mathbf{x} = (y, z)$ to point $\mathbf{x}' = (y', z')$ and $\hat{H}(\mathbf{x})$ is the quantum mechanical Hamiltonian of the type (1)

$$\hat{H}(\mathbf{x}) = \frac{1}{2m}(\mathbf{p} + \mathbf{A})^2 + V(\mathbf{x}), \tag{30}$$

where we have chosen

$$\mathbf{A} = (-B_0 y \cos\theta + B_0 z \sin\theta, 0, 0), \tag{31}$$

$\mathbf{p} = -\mathrm{i}\boldsymbol{\nabla}$ and $\hat{H}^\dagger(\mathbf{x})$ is obtained from $\hat{H}(\mathbf{x})$ by changing the sign of the vector potential.

Multiplying equation (28) by $G(\mathbf{x}', \mathbf{x}, E)$ and equation (29) by $\psi(\mathbf{x})$, subtracting these equations and integrating over a volume V, encircling the point $\mathbf{x}'$, one obtains:

$$\psi(\mathbf{x}') = \frac{1}{2m} \int_V \mathrm{d}\mathbf{x} \, \big(\psi(\mathbf{x})(\boldsymbol{\nabla} + \mathrm{i}\mathbf{A}(\mathbf{x}))^2 G(\mathbf{x}', \mathbf{x}) - G(\mathbf{x}', \mathbf{x})(\boldsymbol{\nabla} - \mathrm{i}\mathbf{A}(\mathbf{x}))^2 \psi(\mathbf{x})\big). \tag{32}$$

Since the vector potential (31) has been chosen in the gauge $\partial_\mu A_\mu = 0$ the integrand can be written as $\partial_\mu J_\mu$ and the current J_μ is given by:

$$J_\mu(\mathbf{x}) = \frac{1}{2m} \big(\psi(\mathbf{x})\partial_\mu G(\mathbf{x}', \mathbf{x}) - G(\mathbf{x}', \mathbf{x})\partial_\mu \psi(\mathbf{x}) + 2\mathrm{i}A_\mu(\mathbf{x})G(\mathbf{x}', \mathbf{x})\psi(\mathbf{x})\big).$$

Stokes' theorem permits one to replace the integral over the volume by one over the surrounding closed boundary. Let us choose this boundary of integration to be restricted from one side by the LH wall and from the other side by an arbitrary surface very far from the point of tunneling ($\mathbf{x} = 0$). Since the contribution from this (infinitely removed) surface tends to zero in the semiclassical limit (for the retarded Green function) one concludes that the wave function inside the QW is given by the following integral (in 2 dimensions):

$$\psi(\mathbf{x}) = \frac{1}{2m} \int \mathrm{d}\mathbf{q}(G(\mathbf{x}, \mathbf{q})\partial_z \psi_1(\mathbf{q}) - \psi_1(\mathbf{q})\partial_z G(\mathbf{x}, \mathbf{q})), \tag{33}$$

where $\mathbf{q}$ is the vector with coordinates $(y, 0)$ and the boundary values of $\psi_1(\mathbf{q})$ are given by equation (27). In Appendix A we shall show that this expression corresponds to the first order perturbation theory result on the tunneling amplitude similar to the perturbation theory used by Bardeen in [17].

To use this formula one has to compute the exact Green function (29). Assuming that the QW is sufficiently wide one can safely use the standard semiclassical approximation (see *e.g.* [3]) for the 2d Green function $G_2(\mathbf{x}', \mathbf{x}, E)$. In this approximation the 2d Green function is represented by a sum over all classical trajectories in the (y, z) plane connecting two points $\mathbf{x}$ and $\mathbf{x}'$:

$$G_2(\mathbf{x}', \mathbf{x}, E) = \sum_j G_j(\mathbf{x}', \mathbf{x}, E), \tag{34}$$

where $G_j(\mathbf{x}',\mathbf{x},E)$ is the semiclassical contribution of an individual classical trajectory (labeled by j)

$$G_j(\mathbf{x}',\mathbf{x},E)=\frac{m}{\sqrt{k_2k_1}}A_jD_j\exp\Big(\mathrm{i}S_j(\mathbf{x}',\mathbf{x},E)-\mathrm{i}\frac{\pi}{2}\mu_j\Big). \tag{35}$$

$S_j(\mathbf{x}',\mathbf{x},E)$ is the classical action calculated along the classical trajectory (j) connecting initial and final points, μ_j is the Maslov index for this trajectory which equals the number of conjugate or focal points counted along the trajectory, and A_j is a prefactor

$$A_j=\frac{1}{\mathrm{i}(2\pi\mathrm{i})^{1/2}}\left|\frac{\partial^2 S_j}{\partial t_1\partial t_2}\right|^{1/2}. \tag{36}$$

Here k_2 and k_1 are the modulus of the full momentum, t_2 and t_1 are the coordinates perpendicular to the trajectory in the final and initial point. In actual calculations it is convenient to express second derivatives of the action *via* the elements of the monodromy matrix [3,20]. The latter is defined as the matrix $M=m_{ij}$ connecting the values of the coordinate and the conjugate momentum in the plane perpendicular to a given trajectory in the final and initial points:

$$\begin{pmatrix} t\\ p_t\end{pmatrix}_{\rm final}=\begin{pmatrix} m_{11} & m_{12}\\ m_{21} & m_{22}\end{pmatrix}\begin{pmatrix} t\\ p_t\end{pmatrix}_{\rm initial}. \tag{37}$$

The monodromy matrix can, in principle, be computed from the classical equations of motion linearized in the vicinity of a given trajectory and its importance comes mainly from the fact that their matrix elements are connected by second derivatives of the classical action $S(t_2,t_1)$ [3,20]:

$$\begin{aligned}\frac{\partial^2 S(t_2,t_1)}{\partial t_1^2}&=\frac{m_{11}}{m_{12}},\\ \frac{\partial^2 S(t_2,t_1)}{\partial t_2\partial t_1}&=-\frac{1}{m_{12}},\\ \frac{\partial^2 S(t_2,t_1)}{\partial t_2^2}&=\frac{m_{22}}{m_{12}}.\end{aligned} \tag{38}$$

The formulae (34–38) are the standard semiclassical expressions for the Green function. In our case, nevertheless, two modifications have to be made in order to arrive at a form which is useful for our problem. First, our Green function describes motion inside a well whose walls have a finite width. Therefore after each reflection it is necessary to multiply the above expression by the reflection coefficient similar to (21). In the leading order of the semiclassical approximation it just gives a reflection phase which is different from standard ones like those corresponding to Dirichlet or Neumann boundary conditions. Later we shall see, in the case of extremely clean devices, that differences of the modulus of the reflection coefficient from unity will be important. Second, in real structures the motion of an electron is always perturbed by impurities and by various inelastic processes which induce an effective damping to the contribution of classical motion. In a reasonable approximation (see *e.g.* [22]) it can be modeled by adding a small imaginary part Γ_0 to the energy which is equivalent to the multiplication of the expression (35) by an additional damping factor $\exp(-\Gamma_0 T_j)$ where T_j is the time of motion along the trajectory (j) and $1/\Gamma_0$ plays the role of the elastic mean free time for motion in the quantum well. In the following we ignore the difference between various kinds of mean free paths and in particular the difference between the mean value of the Green function and the product of the two Green functions which can be important in describing the real experiments [22]. This is an over-simplified approximation and further investigations on this subject are desirable.

Therefore each term in equation (34) should be multiplied by an effective damping factor

$$D_j=r_j\exp(-\Gamma_0 T_j), \tag{39}$$

where r_j is the total reflection coefficient. The existence of the damping will give preference, in the final result, to orbits that naturally have the shortest length.

The calculation of the Green function when one of its arguments is on the boundary of the QW (or very close to it) requires special attention. In this case there are 2 different contributions. The first corresponds to a trajectory with momentum $p_z>0$ which does not hit the LH wall. (We assume that the region of the QW lies at $z\geq 0$.) The second contribution comes from a trajectory which has the same initial conditions as the first one but with a z-momentum of opposite sign, $p_z<0$. This trajectory is reflected from the boundary and then follows a path very close to the first trajectory (provided the initial point is near the boundary). Of course the contribution of the second trajectory has to be multiplied by the reflection coefficient. Therefore

$$G(\mathbf{x},\mathbf{q})|_{z'=0}=(1+r_1)G_j(\mathbf{x},\mathbf{q}_0), \tag{40}$$

and

$$\frac{\partial}{\partial z'}G(\mathbf{x},\mathbf{q})|_{z'=0}=-\mathrm{i}p_z(1-r_1)G_j(\mathbf{x},\mathbf{q}_0), \tag{41}$$

where r_1 is the reflection coefficient from the LH wall, $\mathbf{q}=(y,z')$, and $G_j(\mathbf{x},\mathbf{q})$ is the contribution of one trajectory starting from the point $\mathbf{q}_0=(y,0)$ with $p_z>0$ and ending at the point $\mathbf{x}$.

6 Motion in the quantum well

The explicit expression for the Green function and the value of the wave function in the vicinity of the LH barrier (27) permits one to make a semiclassical computation of the wave function at any point inside the QW. A difficulty appears here because in equations (28, 29) it was assumed that the function $\psi(\mathbf{x})$ is an eigenfunction of the Hamiltonian (30) but the function (27) is not an exact eigenfunction but a variational approximation to it. Even if it can give a good approximation to the exact eigenvalue in the emitter well, its closeness to the corresponding eigenfunction is questionable. Therefore, by using the simple function (27) one can, in the best case, obtain an approximate answer. This point is worth further investigation but for simplicity we shall continue to use the function (27).

Taking into account that at the LH wall $\chi_1(0) = 1/\sqrt{k_z}$, $\partial\chi_1/\partial z(0) = \mathrm{i}k_z\chi_1(0)$ where k_z is the value of the z component of the momentum at $z = 0$ one obtains:

$$\psi(\mathbf{x}) = \frac{\mathrm{i}\sqrt{k_z}C}{2m}\int \psi_0(y)\left(G(\mathbf{x},y) + \frac{\mathrm{i}}{k_z}\partial_z G(\mathbf{x},y)\right)\mathrm{d}y. \tag{42}$$

The next step is to substitute the Green function (34) into this expression. The resulting expression gives $\psi(\mathbf{x})$ as a sum over all classical trajectories (j) connecting the initial point $\mathbf{q} = (y, 0)$ with the final point $\mathbf{x} = (y_\mathrm{f}, z_\mathrm{f})$:

$$\psi(\mathbf{x}) = \sum_j \int w_j(y) G_j(\mathbf{x}, y)\mathrm{d}y. \tag{43}$$

Here we have denoted by $G_j(\mathbf{x}, y)$ the contribution (35) to the Green function from a classical trajectory (j) which starts from the point $\mathbf{q} = (y, 0)$ with initial momentum $\mathbf{p}(j) = (p_y(j), p_z(j))$ and ends in the fixed point $\mathbf{x}$ and (see Eqs. (40, 41))

$$w_j(y) = \mathrm{i}\frac{C}{2m} v_j \sqrt{p_z(j)}\psi_0(y), \tag{44}$$

where

$$v_j = (1 - r_1)\sqrt{p_z(j)/k_z} + (1 + r_1)\sqrt{k_z/p_z(j)}.$$

Here $p_z(j)$ is the initial z-momentum of trajectory j and $k_z = k(0)$ with $k(z)$ from the initial wave function.

This expression is correct provided either (i) $\psi_1(y, 0)$ and $\partial_z\psi_1(y, 0)$ are boundary values of a certain exact solution of the Schrödinger equation (otherwise the Stokes theorem cannot be applied), or (ii) when they are considered as being exact which is usually the case in numerical calculations based on the simplified model of resonant tunneling discussed below. If, as usual, these boundary values are only an approximation to an exact solution it is quite difficult to estimate an error in v_j without additional numerical calculations. One can for example argue that, just after the tunneling through the first barrier, the electron should be represented only as an out-going wave which means that in the exact solution the in-coming component of the current has to vanish. In such an approximation only one type of trajectory will contribute and

$$v_j = \sqrt{p_z(j)/k_z} + \sqrt{k_z/p_z(j)}.$$

Both expressions equal 2 under a natural condition $|p_z(j) - k_z| \ll |p_z(j)|$ and we think that this value is a good zeroth order approximation for this quantity (in the sense that it does not require additional numerical computations).

Without the simplifying assumption (26)

$$C\psi_0(y)/\sqrt{k_z} = \psi_1(y, 0) \quad \text{and} \quad k_z = \partial \log\psi_1(y, 0)/\partial z$$

are just the boundary values of the initial wave function on the LH barrier to be determined either numerically or by more refined methods of multidimensional tunneling.

As each G_j is proportional to $\exp(\mathrm{i}S_j)$ in the semiclassical limit the integration over $\mathbf{q}$ can be done by the saddle point method. Assuming that the boundary function $\psi_0(y)$ and other quantities (such as the tunneling probabilities) do not change noticeably with respect to changes in the Green function, one concludes that in such an approximation the dominant contribution to the above integrals will be given by points y_0 for which

$$\frac{\partial S}{\partial y}|_{y_0} = 0. \tag{45}$$

In other words only trajectories which are perpendicular to the plane $z = 0$ will give a strong contribution. As the QW is assumed wide, one can suppose that a small change in y at $z = 0$ will create a large change in the generating function and we will assume that $D_j \gg B$ (see Eq. (47)). In the following chapter we will see that this property is satisfied strictly speaking only if the Lyapunov exponent of the periodic orbit is large and the orbit is strongly unstable. In this case a small change in y effects largely the action and the Green function oscillates sufficiently rapidly so that the initial state is just a smoothly varying function. In this case the integral over the deviation from the saddle point will cutoff on the scale of the quadratic form in the exponent (*i.e.* of the order of $1/\sqrt{|D_j|}$) and one can extract all factors like ψ_0 just at the value of coordinates corresponding to the periodic orbits considered.

Whereas this treatment is valid in the strong semiclassical limit this assumption may break down for stable or nearly stable orbits. We shall treat this problem in Section 7.

Under the above assumption the integration in the quadratic approximation gives

$$\psi(\mathbf{x}) = \sum_j W_j G_j(\mathbf{x}, \mathbf{q}_0(j)), \tag{46}$$

where

$$W_j = w_j(y_0)\sqrt{\frac{2\pi}{|D_j|}}\mathrm{e}^{\mathrm{i}\pi s_j/4}, \tag{47}$$

and $D_j = \partial^2 S/\partial y^2$ and $s_j = \text{sign } D_j$.

This formula has a clear physical meaning. The wave function at a point inside the QW is represented as a sum over all classical trajectories which start from the plane $z = 0$ with momentum perpendicular to this plane and end in the point of reference. The relative importance of different contributions is govern by the wavefunction in the first well. The amplitude of the tunneling can be computed from knowledge of the imaginary part of the quasibound state in the first well (which in our approximation depend only on $E_{(z)}$).

The knowledge of the wave function (43) permits us to compute the current $\mathbf{j}_{\mathrm{i}}(\mathbf{x}_{\mathrm{f}}) = \mathbf{j}_{\mathrm{i}}(y, d)$ at the second interface of the QW (*i.e.* at the RH wall):

$$\mathbf{j}_{\mathrm{i}}(\mathbf{x}_{\mathrm{f}}) = -\frac{\mathrm{i}}{2m}(\psi^*(\mathbf{x}_{\mathrm{f}})\boldsymbol{\nabla}\psi(\mathbf{x}_{\mathrm{f}}) - \boldsymbol{\nabla}\psi^*(\mathbf{x}_{\mathrm{f}})\psi(\mathbf{x}_{\mathrm{f}})). \quad (48)$$

When the electron hits the second barrier it has a probability of tunneling through the wall. In the same approximation as before the current after the barrier, $(\mathbf{j}_{\mathrm{f}})$, differs from the current before it, $(\mathbf{j}_{\mathrm{i}})$, by a transmission coefficient through this barrier (t_2):

$$\mathbf{j}_{\mathrm{f}} = |t_2|^2\mathbf{j}_{\mathrm{i}}. \quad (49)$$

The total imaginary part, Γ, of the energy of a quasi-bound state in the emitter well is equal to the total current after the second barrier (see (15)). Assuming once more that the tunneling probability depends only on the z component of momentum this total current is given by an integral over all final positions at $z = d$:

$$\Gamma = \int_S \mathrm{d}\boldsymbol{\sigma}_2\mathbf{j}_{\mathrm{i}}|t_2|^2. \quad (50)$$

Substituting here the expression (43) for the wave function one gets

$$\Gamma = \sum_{j,k}\int \mathrm{d}y\mathrm{d}y' w_{jk}(y, y')\int G_j(y_{\mathrm{f}}, y)\bar{G}_k(y_{\mathrm{f}}, y')\mathrm{d}y_{\mathrm{f}}|t_2|^2, \quad (51)$$

where

$$w_{jk}(y, y') = \frac{1}{2m}(p_z^{(\mathrm{f})}(j) + p_z^{(\mathrm{f})}(k))w_j(y)\bar{w}_k(y')$$

and $G_j(y_{\mathrm{f}}, y)$ is the contribution (35) of a trajectory (j) which starts at the point $(y, 0)$ and ends at the point (y_{f}, d).

In the semiclassical approximation G_j is proportional to $\exp(\mathrm{i}S_j/\hbar)$ and in the formal limit $\hbar \to 0$ it is natural to perform the integration over all variables by the saddle point method. Assuming as above that the boundary function $\psi_0(y)$ and other quantities are smooth in the scale of noticeable changes of the Green function, one concludes that in such an approximation the dominant contribution to the above integrals will be given by trajectories in the vicinity of saddle-points trajectories for which the following three conditions are fulfilled:

$$\frac{\partial S_j(y_{\mathrm{f}}, y)}{\partial y_{\mathrm{f}}} - \frac{\partial S_k(y_{\mathrm{f}}, y')}{\partial y_{\mathrm{f}}} = 0, \quad (52)$$

and

$$\frac{\partial S_j(y_{\mathrm{f}}, y)}{\partial y} = 0, \; \frac{\partial S_k(y_{\mathrm{f}}, y')}{\partial y'} = 0. \quad (53)$$

The first equation means that saddle point trajectories (labeled here by j and k) should have the same y component of momentum: $p_y^{(\mathrm{f})}(j) = p_y^{(\mathrm{f})}(k)$. The equality of the p_z momenta for these trajectories then follows from energy conservation. But two classical trajectories passing through the same point (y_{f}) and having the same momenta at this point can be either (i) exactly the same trajectory or (ii) two different paths on the same classical trajectory (see Fig. 3). We stress that this is a consequence of the integration over y_{f}.

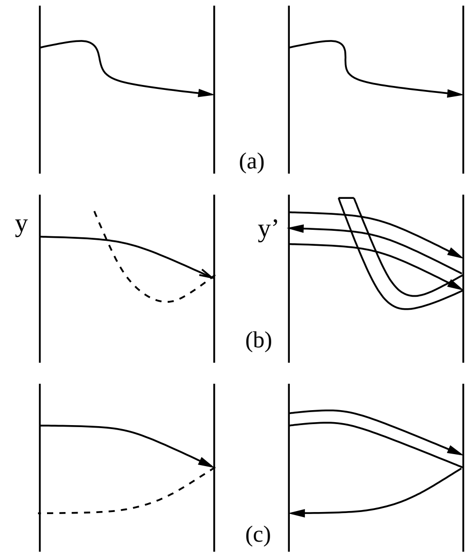

Fig. 3. Different possibilities for trajectories which give a large contribution to the tunneling current in the saddle point approximation. All trajectories are perpendicular to the first wall at points y and y'. (a) 2 generic trajectories, (b) 2 different paths on a periodic trajectory when $y = y'$, (c) 2 different paths on a periodic trajectory when $y \neq y'$. In cases (b) and (c) one can add an arbitrary number of repetitions along the periodic trajectory.

The second pair of saddle point equations (53) (valid under the assumption that the initial wave function is smooth) signifies that the saddle point trajectories should have zero y component of momentum in both points at the LH wall (*i.e.* they have to be perpendicular to the plane $z = 0$). The combination of these conditions leads to the important conclusion that in the strict semiclassical limit the tunneling current or probability of decay is divided into two distinct contributions:

$$\Gamma = \Gamma_{(\mathrm{Weyl})} + \Gamma_{(\mathrm{osc})}. \quad (54)$$

The first term corresponds to the interference of an arbitrary trajectory perpendicular to the plane $z = 0$ with itself (see Fig. 3a) and it is given by equation (51) with $j = k$ while the second one is the result of interference between different trajectories $j \neq k$, both of them belong to a periodic trajectory with zero initial y-momentum (see Figs. 3b and 3c).

The first term has no quick dependence on the external fields and we shall refer to it as the Weyl (or diagonal) contribution because it plays a role similar to the Weyl term in the usual Gutzwiller trace formula. This contribution gives a smooth background and in real experiments is effectively washed out by taking the second derivative of the current. We shall discuss it later.

The second term is denoted by $\Gamma_{(\mathrm{osc})}$. It includes contributions from different paths on the same *periodic* trajectory which connects both walls and is perpendicular to the LH wall (see Figs. 3b and 3c). In this case there is an interference between different terms in the family of trajectories attaching initial and final points but stationary phase considerations select only a special type of classical orbits. For clarity we repeat the above arguments and organize the details in the following scheme:

- The cancelation of linear terms in the exponential of (51) coming from the stationary phase condition on the final point $y^{(\mathrm{f})}$ selects only orbits with the same value of final y momentum.
- Assuming that the initial function ψ_0 is smooth, the integration over the initial position selects only trajectories with initial y-momentum equal to zero.
- These two conditions together show that the dominant contribution to the tunneling current will come from classical trajectories in the vicinity of *periodic* trajectories which hit both LH and RH walls and are perpendicular to the LH one. Due to the last condition these orbits are self-retracing.
- In general for a (self-retracing) periodic orbit (p) there can exist l points of reflection at $z = d$ and up to 2 points at $z = 0$. In this case the periodic orbit gives rise to l or $2l$ saddle points, each of them has to be taken into account. Every time an electron hits the second wall it can tunnel through but the tunneling probability t_2, in general, is different for each final point.
- The classical trajectories which give the dominant contribution to the resonant tunneling are built from a segment of a periodic orbit which hits both walls plus an arbitrary number of loops around this periodic orbit. We shall call the first segment of this trajectory an orbit with $n = 0$ loops (even if it is not a loop). All other trajectories make an integer $n > 0$ number of loops.
- The sum over trajectories j and k in (51) becomes a sum over primitive periodic orbits with $p_y(z = 0) = 0$, labeled later by j, and over an integer l for the number of times that this orbit hits the RH and LH walls. Finally the integers, n and m, denote the repetition numbers of periodic orbits.
- For periodic orbits with $y = y'$ as in Figure 3b, the difference of actions equals an integer times the action of the periodic orbit (S_p) but for orbits with $y \neq y'$ as in Figure 3c, this difference is a half-integer times S_p.

Applying the above results one gets

$$\Gamma_{(\mathrm{osc})} = \sum_j \Gamma_j |\psi_0(y_0(j)|^2 |t_2|^2 \sum_{m\neq n} \frac{R^{n+m}}{(m_{12}(m)m_{12}(n))^{1/2}} \times \int \mathrm{d}y\mathrm{d}y'\mathrm{d}y_{\mathrm{f}} \exp\Big[\mathrm{i}\Big(S_n(y_{\mathrm{f}}, y) - S_m(y_{\mathrm{f}}, y') + \frac{\pi}{2}(\mu_n - \mu_m)\Big)\Big], \quad (55)$$

and

$$R = \mathrm{e}^{-\Gamma_0 T_p} r_1 r_2.$$

Here the factors r_1 and r_2 are the total reflection coefficient at the LH and RH walls. The factor $\exp(-\Gamma_0 T_p)$ is associated with inelastic processes in the QW (see the discussion after Eq. (38)). Γ_j is defined by the expression

$$\Gamma_j = \frac{\Gamma_1}{8\pi} |v_j|^2. \quad (56)$$

In this formula $m_{ij}(n)$ are the elements of the monodromy matrix $M(n)$ for the full trajectory with n loops. If we denote the monodromy matrix for the trajectory with $n = 0$ loops by M_0 and the monodromy matrix for the periodic trajectory by M_p the total monodromy matrix will be

$$M(n) = M_0 M_p^n. \quad (57)$$

Note that the matrix M_p is defined with respect to the first wall.

To perform the integration over final and initial values of y coordinate we expand the actions in the exponent around each stationary point on both the LH and RH walls up to second order with deviations from the saddle points $\delta y_1 = \delta y$, $\delta y_2 = \delta y'$, $\delta y_3 = \delta y_{\mathrm{f}}$. It gives

$$\Phi(\delta y_k) = \frac{1}{2} A_{kl} \delta y_k \delta y_l, \quad (58)$$

where the matrix A_{kl} is a 3×3 matrix constructed from the second derivatives of the actions at the saddle point

$$A_{kl} = \begin{pmatrix} \frac{\partial^2 S_n}{\partial y^2} & \frac{\partial^2 S_n}{\partial y \partial y_{\mathrm{f}}} & 0 \\ \frac{\partial^2 S_n}{\partial y \partial y_{\mathrm{f}}} & \frac{\partial^2 S_n}{\partial y_{\mathrm{f}}^2} - \frac{\partial^2 S_m}{\partial y_{\mathrm{f}}^2} & -\frac{\partial^2 S_m}{\partial y' \partial y_{\mathrm{f}}} \\ 0 & -\frac{\partial^2 S_m}{\partial y' \partial y_{\mathrm{f}}} & -\frac{\partial^2 S_m}{\partial y'^2} \end{pmatrix}. \quad (59)$$

After the integration over δy_j one obtains that

$$(m_{12}(m)m_{12}(n))^{-1/2} \times \int \mathrm{d}y\mathrm{d}y'\mathrm{d}y_{\mathrm{f}} \exp(\mathrm{i}S_n(y_{\mathrm{f}}, y) - \mathrm{i}S_m(y_{\mathrm{f}}, y')) = (2\pi)^{3/2} (S_{nm})^{-1/2} \exp\Big(\mathrm{i}(n-m)S_p + \mathrm{i}\frac{\pi}{4}\Big), \quad (60)$$

where the prefactor

$$S_{nm} = -\det A\; m_{12}(n) m_{12}(m). \quad (61)$$

To obtain the explicit form of the prefactor S_{nm} it is convenient to express the second derivatives of the action through the monodromy matrix elements as in (63). Simple calculation gives

$$S_{nm} = m_{21}(n)m_{11}(m) - m_{11}(n)m_{21}(m).$$

But this expression can be written as the (21) matrix element of the matrix

$$M^{-1}(m)M(n),$$

from which it is evident that S_{nm} does not depend on the matrix M_0 in (57) and

$$S_{nm} = m_{21}^{(p)}(n-m), \tag{62}$$

where $m_{21}^{(p)}(r)$ is the (21) monodromy matrix element for r repetitions of the primitive periodic orbit.

It easy to show that the n-fold application of the monodromy matrix M has the following form

$$M^n = \begin{pmatrix} m_{11}(n) & m_{12}(n) \\ m_{21}(n) & m_{22}(n) \end{pmatrix}, \tag{63}$$

where

$$\begin{aligned} m_{11}(n) &= a\lambda^n + b\lambda^{-n}, \\ m_{12}(n) &= \frac{\lambda^n - \lambda^{-n}}{\lambda - \lambda^{-1}} m_{12}, \\ m_{21}(n) &= \frac{\lambda^n - \lambda^{-n}}{\lambda - \lambda^{-1}} m_{21}, \\ m_{22}(n) &= b\lambda^n + a\lambda^{-n}, \\ a &= \frac{\lambda - m_{11}}{\lambda - \lambda^{-1}}, \\ b &= \frac{\lambda - m_{22}}{\lambda - \lambda^{-1}}. \end{aligned}$$

Here λ and λ^{-1} are eigenvalues of the monodromy matrix for a primitive periodic orbit.

Therefore

$$S_{nm} = m_{21} \frac{\lambda^{m-n} - \lambda^{n-m}}{\lambda - \lambda^{-1}}.$$

For periodic orbits with $y \neq y'$ as in Figure 3c, instead of equation (57) one has

$$M(n) = M_0 M_{p/2}^{2n} \quad \text{and} \quad M(m) = M_0 M_{p/2}^{2m+1},$$

where $M_{p/2}$ is the monodromy matrix for half of the primitive periodic orbit. The modifications to equation (62) for this case are evident.

Let us now consider the phase factor which comes after the action. This term is made up of three contributions which we write in the following way

$$\sigma_t^{k\to l}(n,m) = \mu_t(n) - \mu_t(m) + \mathrm{sgn}(\lambda_t(n,m)). \tag{64}$$

The first (second) term gives the count for the number of conjugate points for member n (respectively m) in the family of periodic trajectories. The third term comes from integration of the quadratic form and is given by

$$\mathrm{sgn}(\lambda_t(n,m)) = N_+/2 - N_-/2. \tag{65}$$

In the previous equation $N_+(N_-)$ are the number of positive (negative) eigenvalues in the quadratic form evaluated at the stationary point at $z = 0$. In our case the quadratic form can be expressed as a matrix with three eigenvalues and $N_+ + N_- = 3$. *A priori* it is not obvious that $\sigma_t(n,m)$ is invariant with respect to changes of starting and final point that are connected by an integral number of loops. A first observation that will clarify the problem is that the number of conjugate points along a periodic orbit does not scale with the number of loops executed. In particular it would be possible to count M such points during one traversal and a number $N \neq M$ on the following traversal. We begin by making a count of the number of conjugate points for one loop. We then follow this numerical calculation by computing the same number for subsequent loops from simple knowledge of the monodromy matrix and the count made for the first loop. Furthermore after calculating m traversals one can make another $n-m$ loops, return back to the second wall, and count a fixed number of conjugate points which depends on n and m and not on the difference. On the other hand it is clear that for any other n' and m' such that $n'-m' = n-m$ we will count the same number plus or minus one. It is then easy to show that the third term in equation (64) makes the correct compensation so that, for example, when there is exactly one less conjugate point counted there is exactly one more negative eigenvalue and that when there is exactly one more conjugate point in the count there is exactly one more positive eigenvalue.

Similar arguments were made in [21] to treat the phase that appears in the Gutzwiller formula for the level density. The arguments nevertheless are quite simple and one can always obtain empirical results to assure oneself that the phase factor in (64) is an intrinsic property of the periodic orbit. Furthermore the action S_p evidently scales with the number of repetitions.

Using the above information we can transform the sum over n and m into the sum over $r = (n-m)$ and $(m+n)$. The latter can easily be done and one obtains

$$\begin{aligned} \Gamma_{(\mathrm{osc})} = \sum_p \Gamma_p |t_2^{(\mathrm{tot})}(p)|^2 \frac{1}{1-|R_p|^2} \\ \times \sum_{r=1}^{\infty} \frac{R_p^r}{(m_{21}^{(p)}(r))^{1/2}} \cos\left(rS_p - \frac{\pi}{2}\sigma_p(r) + \mathrm{i}\frac{\pi}{4}\right). \end{aligned} \tag{66}$$

Here

$$\Gamma_p = \left(\frac{\pi}{2}\right)^{1/2} \Gamma_1 |v_p|^2 |\psi_0(y_0(p))|^2 \tag{67}$$

is the tunneling probability through the first wall weighted by the initial wave function at the point of tunneling.

$$|t_2^{(\mathrm{tot})}(p)|^2 = \sum_l |t_2(p,l)|^2 \mathrm{e}^{-2\Gamma_0 T_l}$$

is the total tunneling probability through the second wall given by the sum over all point of reflection with the second wall weighted by the damping factor corresponding to the time of motion on the segment of periodic orbit from the initial point to the lth final point (T_l).

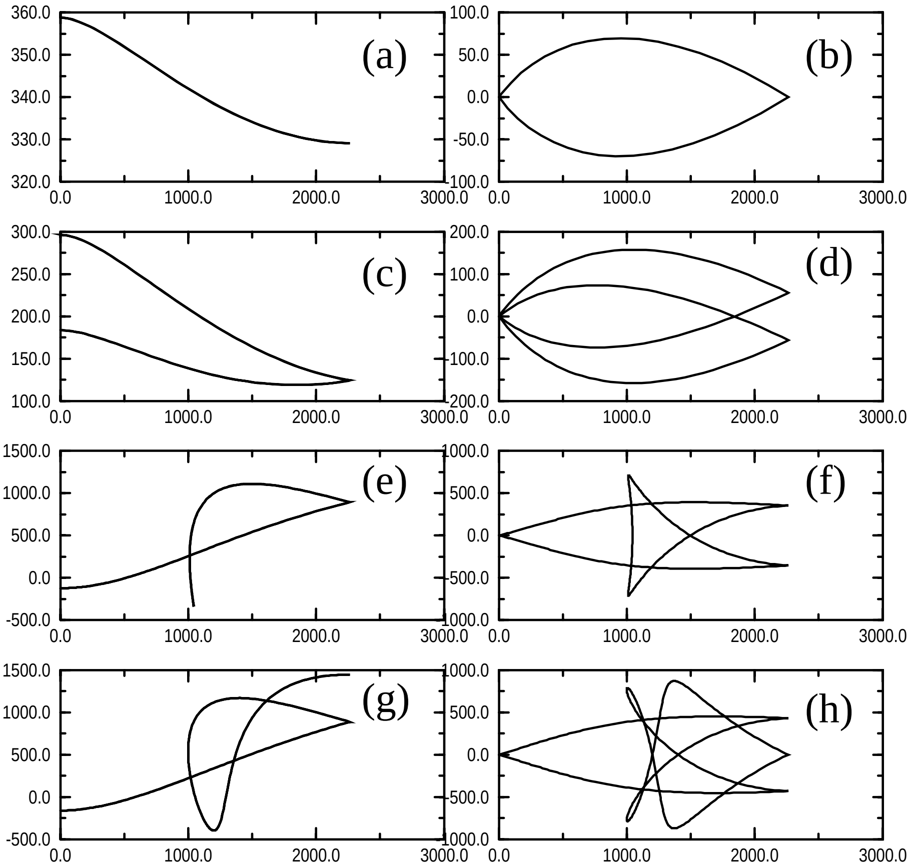

Fig. 4. Short-period orbits in the (z, y) plane (on the left) and in the (z, x) plane (on the right). (a), (b) One bounce periodic orbit. (c), (d) One bounce periodic orbit with two bounces on the LH wall. (e), (f) Two bounce periodic orbit with the same bounce on the RH wall. (g), (h) Three bounce periodic orbit.

The sum above is taken over all primitive periodic trajectories with $p_y(z = 0) = 0$ labeled by (p) and $y_0(p)$ is the y coordinate of initial point on the first wall for periodic orbit (p) (few examples of such trajectories are presented in Fig. 4),

$$R_p = r_{(\mathrm{tot})}(p) \exp(-\Gamma_0 T_p)$$

where $r_{(\mathrm{tot})}(p)$ is the total reflection coefficient with the LH and RH walls for one loop around the given periodic orbit

$$r_{(\mathrm{tot})} = \prod_j r(j).$$

The factor $\exp(-\Gamma_0 T_p)$, where T_p is the period of the trajectory, has been introduced to take into account various inelastic processes in the QW. (For a more careful treatment of the damping processes see *e.g.* [22].) We always consider the tunneling through different points as a noncoherent process.

This formula is the main result of the paper. It expresses the tunneling current as a sum over special periodic trajectories which (i) connect the two walls of the QW and (ii) are perpendicular to the first barrier. The contribution of each of these trajectories contains the factor $\cos(rS_p - \pi\sigma_p(r)/2)$ like in the usual Gutzwiller trace formula but the prefactor is different. First of all it is not a canonical invariant and contains the m_{21} matrix element of the monodromy matrix computed along the first barrier unlike the factor $\lambda + \lambda^{-1} - 2$ which appears in the Gutzwiller trace formula.

The coefficient of proportionality consists of three parts. One is connected with the properties of the tunneling through the first barrier and with the structure of the initial wave function. The second appears due to different inelastic processes and the third equals the probability of tunneling through the second barrier.

It is important to note that all factors depend on the chosen periodic trajectory.

There is an interesting limit of this formula. It corresponds to the case of very clean devices where Γ_0 is very small. In this case $R = r_1 r_2$ where r_i are coefficients of reflection. Using the relation $R^2 = 1 - |t|^2$ and assuming that the probability of tunneling through the second barrier is much bigger than through the first one we conclude that $R^2 = 1 - |t_2^{(\mathrm{tot})}|^2$ and equation (66) reduces to

$$\Gamma_{(\mathrm{osc})} = \sum_p \Gamma_p \sum_{r=1}^{\infty} \frac{R_p^r}{(m_{21}^{(p)}(r))^{1/2}} \times \cos\left(rS_p - \frac{\pi}{2}\sigma_p(r) + \frac{\pi}{4}\right). \qquad (68)$$

In Section 8 we shall see that this expression equivalent to the semiclassical approximation resulting from the simplified model of tunneling discussed in [14,15].

Let us now return to the calculation of the Weyl term. It is easy to see that the method used for the computation of $\Gamma_{(\mathrm{osc})}$ can not be applied for $\Gamma_{(\mathrm{Weyl})}$. *E.g.* the prefactor S_{nm} in (61) equals zero when $n = m$. This is not surprising as even for the Gutzwiller trace formula the Weyl contribution comes from short trajectories for which semiclassical approximation cannot be used. In such a case we shall proceed as follows.

Let us fix a classical trajectory which starts perpendicular to the first wall at a point y and after the time $T_l(y)$ crosses the second wall at points $y_{\mathrm{f}}(y,l)$. The index $l = 1, 2, \ldots$ denotes the different points of intersection of this trajectory with the second wall and we write explicitly the dependence of y in order to stress that all these quantities are function only of y. Note that the point y is not fixed contrary to the above-considered case of periodic orbits. The Weyl contribution to the tunneling density is given by the expression similar to equation (55) but with (i) $n = m$ and (ii) the sum over a discrete sum of periodic orbits in (55) is replaced by the integral over y and the sum over all possible points of reflection with the second wall (l):

$$\Gamma_{(\mathrm{Weyl})} = \int \Gamma(y)|\psi_0(y)|^2 \mathrm{d}y\mathrm{d}y' \times \sum_l |t_2(y,l)|^2 r_{\mathrm{tot}}(y,l)\mathrm{e}^{-\Gamma_0 T_l(y)} \frac{1}{m_{12}} \times \int \mathrm{d}y_{\mathrm{f}} \exp\left[\mathrm{i}(S(y_{\mathrm{f}},y) - S(y_{\mathrm{f}},y'))\right]. \quad (69)$$

Assuming that $y' = y + \delta z$, $y_{\mathrm{f}} = y_{\mathrm{f}}(y,l) + \delta y_{\mathrm{f}}$ where δz and δy_{f} are small and expanding the actions up to the second order one obtains that the difference of actions equals

$$-\frac{1}{2}\frac{\partial^2 S}{\partial y^2}\delta z^2 - \frac{\partial^2 S}{\partial y \partial y_{\mathrm{f}}}\delta z \delta y_{\mathrm{f}}.$$

Now the integration over δz and δy_{f} gives $2\pi m_{12}$ which cancels the factor m_{12} in the denominator.

Finally we get

$$\Gamma_{(\mathrm{Weyl})} = 2\pi \int \Gamma(y)|\psi_0(y)|^2 \mathrm{d}y \times \sum_l |t_2(y,l)|^2 r_{(\mathrm{tot})}(y,l)\mathrm{e}^{-\Gamma_0 T_l(y)}. \quad (70)$$

In order to use this formula one has to find a classical trajectory which begins perpendicular to the first wall at the point y and follows it for all points of reflection with the second wall (labeled by l). There is an infinity of such points but the inelastic cut-off in (70) will effectively force the sum to converge. $\Gamma(y)$ (see (67)) is the tunneling probability through the first wall for the trajectory considered weighted by the value of the initial wave function at the point y, $t_2(y,l)$ is the tunneling probability through the second wall at the lth point of reflection, $r_{(\mathrm{tot})}(y,l)$ is the total reflection coefficient for this segment of trajectory, and $T_l(y)$ is the time of motion from the point y to the lth point of reflection.

Assume now that the inelastic damping Γ_0 is absent or is very small and the tunneling through the RH wall is much larger than through the LH wall (*e.g.* $r_1 = 1$). Then to compute Γ_{Weyl} one has to calculate the sum over all possible reflections with the RH wall

$$S = |t(1)|^2 + |r(1)|^2|t(2)|^2 + |r(1)r(2)|^2|t(3)|^2 + \ldots + |\prod_{i=1}^{n} r(i)|^2 |t(n+1)|^2 + \ldots, \quad (71)$$

where $t(i) = t_2(i)$ and $r(i) = r_2(i)$. Using the relation $|t(i)|^2 = 1 - |r(i)|^2$ one can transform the above sum as follows

$$S = 1 - |r(1)|^2 + |r(1)|^2(1 - |r(2)|^2) + |r(1)r(2)|^2(1 - |r(3)|^2) + \ldots = 1. \quad (72)$$

It means that after the sum over all reflections of a classical trajectory with the RH wall the dependence of the tunneling coefficient will disappear as it should from physical considerations and the Weyl contribution (70) is defined merely by the current through the first wall

$$\Gamma_{(\mathrm{Weyl})} = 2\pi \int \Gamma(y)|\psi_0(y)|^2 \mathrm{d}y. \quad (73)$$

7 Next terms of semiclassical expansion

The above mentioned formulae for the tunneling current have been derived in the strict semiclassical limit under the assumption that the initial wave function changes much more slowly than the Green function for motion in the quantum well.

It is easy to check (see (66)) that this requirement is equivalent to the condition

$$\beta \ll \frac{\partial^2 S(y,y')}{\partial y^2} = \frac{m_{11}}{m_{12}}, \quad (74)$$

where $\beta = B\cos\theta$ and the same condition for the second derivative with respect to y'.

It seems that this condition is necessary for any application of semiclassical methods to work because the initial wave function has to be connected with the lowest energy state in the first well which by definition of the semiclassical approximation has to be smooth on a semiclassical scale.

Another way of reasoning is the following. The value of magnetic field in atomic units is always small: (B in a.u.) $= 4.3 \times 10^{-6}$ (B in tesla). On the other hand the second derivative of the action equals the ratio of two monodromy matrix elements: $\partial^2 S/\partial y^2 = m_{11}/m_{12}$, and for chaotic systems there is no reason why this ratio should be particularly small. The usual situation is that for strongly chaotic systems all monodromy matrix elements are of the same order. This ratio may be small for a periodic orbit in a stable region as in this case the transversal energy always remains small. It is a characteristic property of chaotic systems that there is no possibility of having certain parameters small during the motion even if their initial values are small. All quantities after the time of mixing will be ergodically spread over the whole allowed region.

But experimental values of external fields and the sizes of the tunneling diodes sometimes are such that for certain not very unstable orbits the condition of applicability of semiclassical approximation may not be justified (see Fig. 5). Though with increasing the degree of chaoticity the condition (74) will be satisfied (see *e.g.* Fig. 5d), contributions of such orbits can be large and the corrections to the above-derived semiclassical formulae will be of importance.

There exist different types of such corrections (see *e.g.* [23]) but we shall restrict ourselves to the contributions due to the dependence of the initial wavefunction on the starting point[1].

Let the boundary value of the initial wave function be of the form (9)

$$\psi_0(y) = (\beta/\hbar\pi)^{1/4} \exp\left(-\frac{1}{2\hbar}\beta y^2\right), \tag{75}$$

where for simplicity we drop the diamagnetic shift and as above $\beta = B_{\|} = B\cos\theta$. Note the $\hbar$ dependence of the exponent. The main quantity of interest will be the integral of this function with the Green function as in equation (43). Using a semiclassical expression for the Green function (34, 35) one is lead to the computation of the following integral

$$I = \int \exp\left(-\frac{\beta y^2}{2\hbar} + \mathrm{i}\frac{S(y,y')}{\hbar}\right) g(y)\mathrm{d}y, \tag{76}$$

where the function $g(y)$ coming from different prefactors is assumed to be smooth in the scale of $\hbar$. Then in the limit $\hbar \to 0$ one has to apply the saddle point method to the exponent which gives the following equation for the saddle point y_{c},

$$\mathrm{i}\frac{\partial S}{\partial y}\,|_{y=y_{\mathrm{c}}} - \beta y_{\mathrm{c}} = 0. \tag{77}$$

If β is small as was assumed in the previous section this equation reduces to the condition

$$\frac{\partial S}{\partial y}\,|_{y=y_c} = 0,$$

which can be interpreted as the statement that the dominant contribution to the tunneling current comes from trajectories perpendicular to the first wall.

[1] In principle other quantities like the tunneling probabilities may also depend sensibly on the initial conditions of a trajectory. In such cases the construction of the perturbation theory below should be modified.

In general equation (77) should give a complex value for y_{c} and the dominant contribution will be due to complex trajectories. The calculation of complex trajectories though numerically possible is not a simple problem and we propose to treat them by perturbation theory in β.

Let us denote by y_0 the solution of the precedent equation

$$\frac{\partial S}{\partial y}\,|_{y=y_0} = 0.$$

Then the complex solution of equation (77) can be written as a formal series in β,

$$y_c = y_0 + \sum_{n=1}^{\infty}\left(\frac{\beta}{S^{(2)}}\right)^n y_n, \tag{78}$$

the coefficients of which can be easily obtained recursively from equation (77).

In this way one obtains

$$\begin{aligned} y_1 &= -\mathrm{i}y_0, \\ y_2 &= -y_0\left(1 - \frac{S^{(3)}}{S^{(2)}}y_0\right), \\ y_3 &= \mathrm{i}y_0\left(1 - \frac{S^{(3)}}{S^{(2)}}y_0\right)\left(1 - \frac{S^{(3)}}{S^{(2)}}y_0\right) - \frac{\mathrm{i}}{6}\frac{S^{(4)}}{S^{(2)}}y_0^3, \end{aligned} \tag{79}$$

and so on. In these formulas $S^{(n)}$ denotes the nth derivative of the action $S(y, y_{\mathrm{f}})$ with respect to y taken at the point y_0. Knowledge of the complex saddle point permits us to compute the integral (76) in the saddle point approximation

$$I = g(y_{\mathrm{c}})\left(\frac{2\pi\hbar}{\partial^2 S_{\mathrm{tot}}(y_{\mathrm{c}})/\partial y^2}\right)^{1/2} \exp\left(\mathrm{i}\frac{S_{\mathrm{tot}}(y_{\mathrm{c}})}{\hbar} + \mathrm{i}\frac{\pi}{4}\right), \tag{80}$$

where $S_{\mathrm{tot}}(y) = S(y) + \mathrm{i}\beta y^2/2$.

According to the series (78) the action $S_{\mathrm{tot}}(y_{\mathrm{c}})$ can also be expanded in a series of β. Taking into account only the first correction to y_{c} one gets

$$S_{\mathrm{tot}} = S(y_0) - \frac{S^{(2)}}{2}\left(\frac{y_0\beta}{S^{(2)}}\right)^2 + \mathrm{i}\frac{\beta y_0^2}{2},$$

which leads to a small modification of the effective action.

In principle the second and higher terms of the expansion in (78) depend on the third and higher derivatives of the action which unlike the second derivatives cannot be expressed through the monodromy matrix elements and require additional numerical calculations. But in our problem one can argue that the higher derivatives of the action should be small in the vicinity of a big island of stability surrounding a stable or almost stable orbit (exactly where standard semiclassical approximation cannot be applied). The main point is that in such a region the classical dynamics has to be close to being integrable and is generated by a Hamiltonian with a quadratic potential. But in such

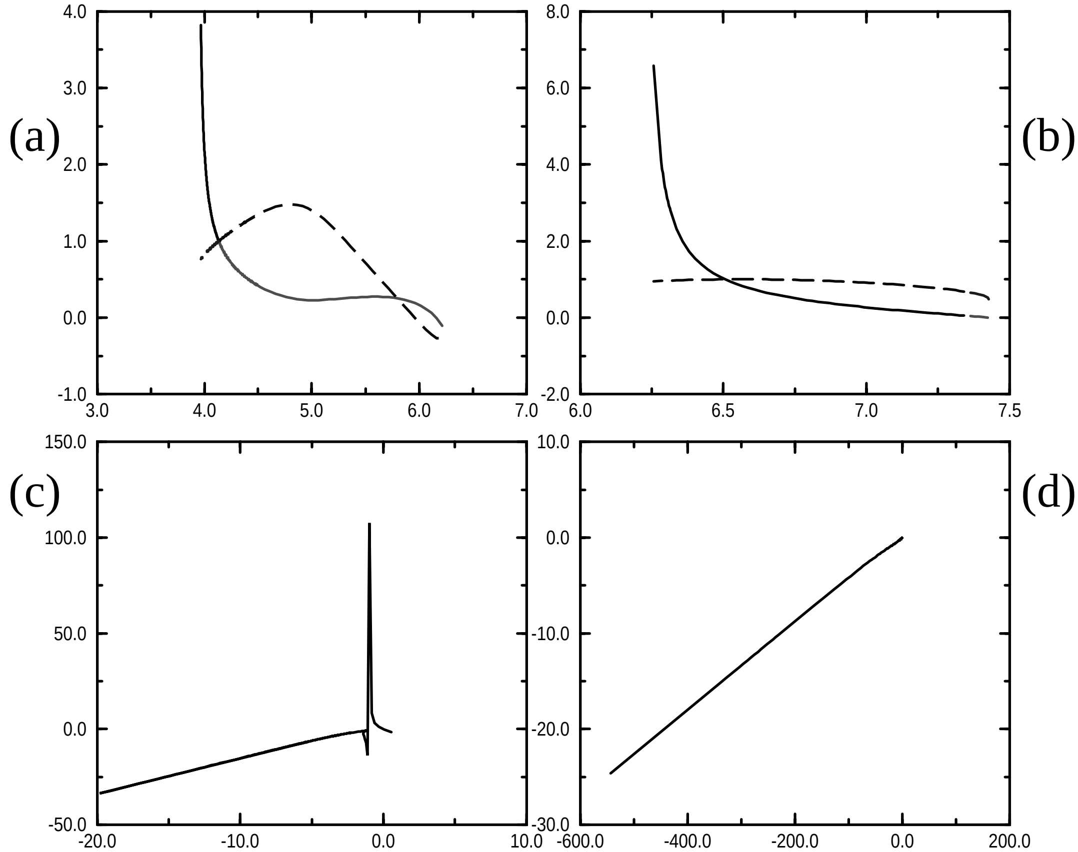

Fig. 5. Semiclassical criterion for the two bounce orbit in Figure 2. Top: $(m_{11}+m_{22})/2$ (solid curve) and m_{12} (jagged curve) at (a) 11° and (b) 34° as a function of $B_\circ \times 10^5$. Bottom: values of $(m_{11}+m_{22})/(2\beta m_{12})$ at (c) 11° and (d) 34° as a function of trace $(m_{11}+m_{22})/2$.

a case the semiclassical Green function for fixed time coincides with the exact Green function and the action is a quadratic function of coordinates [24].

Therefore in the calculation of the triple integral in (51) we shall take into account only quadratic terms of the expansion of the classical action near the point y_0 for which $\partial S/\partial y = 0$ but shall consider the initial wave function ψ_0 in the form (75). We stress that it is not a strict saddle point approximation because the appearance of an effective linear term in (75) necessitates a shift of coordinates and, consequently, a change of the action. This approximation is valid provided the higher order terms of the classical action expansion near the point y_0 are small with respect to the second order terms. Effectively the approximation used is equivalent to the summation of all terms in the series (78) which do not contain derivatives of action higher than second ones.

In such an approximation the triple integral in equation (51) is reduced to the integration of the quadratic form plus the linear terms coming from the initial state

$$I = \int \mathrm{d}\delta\mathbf{y} \exp\left(\frac{\mathrm{i}}{2} A_{ij}\delta y_i \delta y_j - J_i \delta y_i\right), \tag{81}$$

but now the matrix A_{ij} includes the terms coming from the initial wave function

$$A_{kl} = \begin{pmatrix} \dfrac{\partial^2 S_n}{\partial y^2} + \mathrm{i}\beta & \dfrac{\partial^2 S_n}{\partial y \partial y_\mathrm{f}} & 0 \\ \dfrac{\partial^2 S_n}{\partial y \partial y_\mathrm{f}} & \dfrac{\partial^2 S_n}{\partial y_\mathrm{f}^2} - \dfrac{\partial^2 S_m}{\partial y_\mathrm{f}^2} & -\dfrac{\partial^2 S_m}{\partial y' \partial y_\mathrm{f}} \\ 0 & -\dfrac{\partial^2 S_m}{\partial y' \partial y_\mathrm{f}} & -\dfrac{\partial^2 S_m}{\partial y'^2} + \mathrm{i}\beta \end{pmatrix}, \tag{82}$$

and J_i is the vector $\beta(y_0, 0, y_0')$. Performing the integration one obtains a similar result to the one before (see (60))

$$(m_{12}(m)m_{12}(n))^{-1/2} \times \int \mathrm{d}y\mathrm{d}y'\mathrm{d}y_\mathrm{f} \exp(\mathrm{i}S_n(y_\mathrm{f}, y) - \mathrm{i}S_m(y_\mathrm{f}, y')) = (2\pi)^{3/2}(S_{nm})^{-1/2} \exp\left(\mathrm{i}(n-m)S_p + \mathrm{i}\frac{\pi}{4} + \frac{\mathrm{i}}{2} J A^{-1} J\right), \tag{83}$$

where the prefactor

$$S_{nm} = -\det A \; m_{12}(n) m_{12}(m), \tag{84}$$

and A^{-1} is the matrix inverse of the matrix in (82). Simple algebra gives

$$\begin{aligned} S_{nm} &= D(r) \\ &= m_{21}(r) + \mathrm{i}\beta(m_{11}(r) + m_{22}(r)) - \beta^2 m_{12}(r), \end{aligned} \quad (85)$$

and the additional term in the action

$$\Delta S(r) = \frac{1}{2}\beta y_0^2 + \frac{1}{2}\beta y_0'^2 + \frac{1}{2} J A^{-1} J = \frac{1}{2}\beta^2 \times \frac{y_0^2(m_{22}(r)+\mathrm{i}\beta m_{12}(r))+y_0'^2(m_{11}(r)+\mathrm{i}\beta m_{12}(r))+2y_0y_0'}{m_{21}(r)+\mathrm{i}\beta(m_{11}(r)+m_{22}(r))-\beta^2 m_{12}(r)}. \quad (86)$$

Here $r = n - m$ and $m_{ij}(r)$ are the monodromy matrix elements for r repetitions around a primitive periodic orbit.

This result will lead to obvious modifications in the final formula (66) which now will take the form

$$\Gamma_{(\mathrm{osc})} = \frac{1}{2}\sum_p \Gamma_p |t_2^{(\mathrm{tot})}(p)|^2 \frac{1}{1-|R_p|^2} \times \sum_{r=1}^{\infty} \frac{R_p^r}{(D(r))^{1/2}} \Big(\exp \mathrm{i}(rS_p + \Delta S(r) - \frac{\pi}{2}\sigma_p(r)) \Big) + \mathrm{c.c.} \quad (87)$$

We stress once more that in order to obtain this result it is assumed that the derivatives of the classical action of degree 3 and higher are small. Therefore these formulas have to be considered as a simple approximation which (i) does not require information other than monodromy matrix elements and (ii) should be valid when the dynamics near a periodic orbit is close to being integrable.

To perform more consistent calculations it is necessary to compute explicitly complex classical trajectories obeying (77) and in the vicinity of bifurcations take into account higher order terms in the expansion of classical action.

8 Simplified model of resonant tunneling

Up to now we have discussed the sequential theory of tunneling which requires the computation of tunneling probabilities through the barriers of the tunneling diode. In the articles [14,15] a simplified model of resonant tunneling has been discussed which is very convenient from the point of view of numerical calculation. This model is based on the Bardeen transfer matrix [17] (see also Appendix A) according to which the probability of tunneling (or the imaginary part of the energy level) is given by

$$\Gamma = 2\pi \sum_n |W_n|^2 \delta(E - E_n), \quad (88)$$

where E_n denote the exact energy levels in the quantum well and the coefficients W_n are the matrix elements of the current between the wave function in the first well ψ_0 and the exact wave function ψ_n in the quantum well

$$W_n = -\frac{\mathrm{i}}{2m} \int \left(\frac{\partial \bar{\psi}_0(\mathbf{q})}{\partial z} \psi_n(\mathbf{q}) - \bar{\psi}_0(\mathbf{q}) \frac{\partial \psi_n(\mathbf{q})}{\partial z} \right) \mathrm{d}y, \quad (89)$$

and the z-component of the point $\mathbf{q} = (y, z)$ is somewhere inside the barrier.

In references [14,15] for simplicity it was assumed that the height of the barrier was so big that wave functions in the quantum well obey the Dirichlet boundary conditions, $\psi_n(y, 0) = 0$, but we shall use general boundary conditions (defined by the reflection phase in the Green function) as was done in the previous sections.

Using the standard form of the Green function in the energy representation

$$G(\mathbf{x}, \mathbf{x}'; E) = \sum_n \frac{\bar{\psi}_n(\mathbf{x}')\psi_n(\mathbf{x})}{E - E_n + \mathrm{i}\epsilon}, \quad (90)$$

one can express equations (88, 89) through the exact Green function

$$\Gamma = -\frac{1}{2m^2} \int \mathrm{Im}(\hat{\Phi} G(\mathbf{q}, \mathbf{q}'; E)) \mathrm{d}y \mathrm{d}y', \quad (91)$$

where the operator $\hat{\Phi}$ has the form

$$\hat{\Phi} = \left(\frac{\partial \bar{\psi}_0(\mathbf{q})}{\partial z} - \bar{\psi}_0(\mathbf{q}) \frac{\partial}{\partial z} \right) \left(\frac{\partial \psi_0(\mathbf{q}')}{\partial z'} - \psi_0(\mathbf{q}') \frac{\partial}{\partial z'} \right). \quad (92)$$

The semiclassical approximation for the Green function (34, 35) naturally leads to an expression of the current as a sum over all classical trajectories (j) connecting points $(y, 0)$ and $(y', 0)$ on the first wall. Using the separable form of the initial wave function (27) (which was also assumed in [14,15]) and calculating the current at the right border of the first barrier (at point $z = 0$) one obtains

$$\begin{aligned} \Gamma = -\frac{\Gamma_1}{2mk_z} \sum_j \int & \mathrm{d}y \mathrm{d}y' \bar{\psi}_0(y) \psi_0(y') \\ & \times \mathrm{Im}((1 + r_1)k_z + (1 - r_1)p_z)((1 + r_1^*)k_z \\ & + (1 - r_1^*)p_z')G_j(y, y'; E), \end{aligned} \quad (93)$$

where k_z is the momentum coming from the initial wave function, p_z and p_z' are the z-components of momentum at the points $(y, 0)$ and $(y', 0)$ respectively and r_1 is the reflection coefficient from the wall (see (40, 41)). The contribution of an individual classical trajectory, G_j, is given by equation (35).

There are two different types of contribution to this formula. The first one comes from very short trajectories and corresponds to the Weyl term discussed in the previous section. The second term is connected with long classical trajectories which in order to describe tunneling have to hit the RH wall. The latter term describes the oscillatory contribution in the current and is proportional to the integral with a quickly oscillating phase

$$\Gamma_{(\mathrm{osc})} = \sqrt{2\pi \mathrm{i}} \sum_j \Gamma_j \int \mathrm{d}y \mathrm{d}y' \frac{1}{\sqrt{m_{12}}} \times \mathrm{e}^{\mathrm{i}S(y,y') - \mathrm{i}\pi\mu/2} \psi_0(y)\psi_0(y') + \mathrm{c.c.}, \quad (94)$$

where Γ_j is defined in (56) and $S(y,y')$ is the classical action for a trajectory connecting points $(y,0)$ and $(y',0)$ on the LH wall. In the same approximation as above $\psi_0(y)$ is given by the simple Landau-type wave function and everything that was discussed in the previous section can also be applied in this case.

Expanding the action $S(y,y')$ near the points y_0 and y'_0 for which

$$\frac{\partial S(y,y')}{\partial y} |_{y=y_0} = 0, \quad \frac{\partial S(y,y')}{\partial y'} |_{y=y_0} = 0,$$

up to the second order terms one gets a saddle point type integral (93) which reduces to the integration of a quadratic form of 2 variables

$$\int \psi_0(y)\bar{\psi}_0(y') \mathrm{e}^{\mathrm{i}S(y,y')} \frac{1}{\sqrt{m_{12}}} \mathrm{d}y \mathrm{d}y' = \psi(y_0)\psi(y'_0)\mathrm{e}^{\mathrm{i}S(y_0,y'_0)} \times \int \mathrm{d}\delta\mathbf{y} \frac{1}{\sqrt{m_{12}}} \exp\left(\frac{\mathrm{i}}{2} A_{ij}\delta y_i \delta y_j - J_i \delta y_i\right). \quad (95)$$

Here A_{ij} is a 2×2 matrix of the form

$$A_{kl} = \begin{pmatrix} \frac{\partial^2 S}{\partial y^2} + \mathrm{i}\beta & \frac{\partial^2 S}{\partial y \partial y'} \\ \frac{\partial^2 S}{\partial y \partial y'} & \frac{\partial^2 S}{\partial y'^2} + \mathrm{i}\beta \end{pmatrix}, \quad (96)$$

and $J_i = \beta(y_0, y'_0)$.

As usual this integral equals

$$\psi(y_0)\psi(y'_0)\mathrm{e}^{\mathrm{i}S(y_0,y'_0)} \frac{2\pi \mathrm{i}}{\sqrt{m_{12} \det A}} \mathrm{e}^{\mathrm{i}\Delta S}$$

with $\Delta S = \frac{1}{2} J A^{-1} J$.

Simple calculation gives the prefactor

$$D(r) = m_{12} \det A = m_{21} + \mathrm{i}\beta(m_{11} + m_{22}) - \beta^2 m_{12}, \quad (97)$$

and the effective action

$$\Delta S(r) = \frac{\beta^2}{2} \frac{y_0^2(m_{22} + \mathrm{i}\beta m_{12}) + y_0'^2(m_{11} + \mathrm{i}\beta m_{12}) + 2y_0 y'_0}{m_{21} + \mathrm{i}\beta(m_{11} + m_{22}) - \beta^2 m_{12}}, \quad (98)$$

where all monodromy matrix elements are computed for a trajectory starting perpendicularly at the first wall at $(y_0, 0)$ and ending at the point $(y'_0, 0)$. Therefore it is either a self-retracing periodic trajectory or half of such a trajectory in complete agreement with what was obtained in the previous section.

Taking into account all factors we obtain

$$\Gamma_{(\mathrm{osc})} = \frac{1}{2} \sum_p \Gamma_p \sum_{r=1}^{\infty} \Big[\frac{R_p^r}{(D(r))^{1/2}} \times (\exp \mathrm{i}(rS_p + \Delta S(r) - \frac{\pi}{2}\sigma_p(r)) + \mathrm{c.c.} \Big]. \quad (99)$$

Comparing this formula with equations (68, 85, 86, 87) one concludes that the model of references [14, 15] corresponds to the limit of extremely clean device where the tunneling through the second barrier is much bigger than through the first one.

9 Miller type modifications for stable periodic orbits

It is well-known that the Gutzwiller trace formula for the density of states and other semiclassical formulae require a modification for stable periodic orbits. The formal reason for this is the fact that the contribution from a periodic orbit (labeled by p) is proportional to $(\det M_p^n - 1)^{1/2}$ which for a stable orbit (in 2 dimensions) becomes $2\mathrm{i}\sin(n\phi_p/2)$ where $\exp(\pm \mathrm{i}\phi_p)$ are eigenvalues of the monodromy matrix for a primitive periodic orbit and n denotes the number of repetitions around it. It is the summation over n which produces divergences because $\sin(n\phi_p/2)$ can be arbitrarily small for any ϕ_p.

The simplest method to deal with this difficulty was proposed by Miller [25] following a clear physical picture.

Let us write the oscillating part of the density of states as a double sum over primitive periodic orbits and repetitions around it

$$d^{\mathrm{osc}}(E) = \frac{1}{\pi} \sum_p T_p \sum_1^{\infty} \frac{1}{2\mathrm{i}\sin n\phi_p/2} \times \cos n \left(\frac{S_p(E)}{\hbar} - \frac{\pi}{2}\mu_p \right). \quad (100)$$

The Miller modification corresponds

(i) to the formal expansion of the expression

$$\frac{1}{2\mathrm{i}\sin(n\phi/2)} = \frac{1}{\mathrm{e}^{\mathrm{i}n\phi/2} - \mathrm{e}^{-\mathrm{i}n\phi/2}} = \sum_{m=0}^{\infty} \mathrm{e}^{-\mathrm{i}\phi n(m+1/2)}, \quad (101)$$

(ii) rewriting the density of states in the form

$$d^{\mathrm{osc}}(E) = \frac{1}{2\pi\hbar} \sum_p T_p \sum_{m=0}^{\infty} \sum_{n=1}^{\infty} \mathrm{e}^{\mathrm{i}n\Phi_p} + \mathrm{c.c.}, \quad (102)$$

where

$$\Phi_p = S_p/\hbar - \frac{\pi}{2}\mu_p - \phi_p(m + 1/2)$$

(iii) performing the summation over n using the relation

$$\sum_{n=-\infty}^{\infty} \mathrm{e}^{\mathrm{i}n\phi} = 2\pi \sum_{N=-\infty}^{\infty} \delta(\phi - 2\pi N).$$

This scheme leads to the conclusion that the density of states in the vicinity of a stable periodic orbit (p) is equal to the sum of δ-functions

$$d_p(E) = \frac{T_p}{\hbar} \sum_N \sum_{m=0}^{\infty} \delta\left(\frac{S_p(E)}{\hbar} - \phi_p\left(m + \frac{1}{2}\right) - \frac{\pi}{2}\mu_p - 2\pi N\right). \tag{103}$$

Introducing the frequency $\omega_p = \phi_p/T_p$ the sum within semiclassical accuracy can be rewritten as follows

$$d_p(E) = \sum_{N,m} \delta(E - E_{N,m}), \tag{104}$$

where $E_{N,m}$ are defined by the implicit relation

$$S_p(E_{N,m} - \epsilon_\perp(m)) = 2\pi\hbar(N + \mu_p/4), \tag{105}$$

and $\epsilon_\perp(m) = \hbar\omega(m + 1/2)$.

This relation means that in the vicinity of a stable periodic orbit the motion is integrable and the Hamiltonian splits up into 2 integrable Hamiltonians. One corresponds to a harmonic oscillator in the direction perpendicular to the trajectory with frequency ω and the second to a motion along the trajectory and with energy $\epsilon_\parallel = E - \epsilon_\perp$. Equation (105) is just the WKB quantization condition for this longitudinal motion. In such an interpretation the number m in equation (103) has the meaning of a perpendicular quantum number and labels the possible quantum state in the direction perpendicular to the trajectory. If the island of stability is finite the summation over m can not go to ∞ as in equation (103) but has to include only a finite number of states and the maximum number of such states can be estimated from an area of the island.

In the article [15] similar ideas were applied to the tunneling current through the resonant diode. Namely it was assumed that if the island of stability is sufficiently big, one can approximate the exact wave function in equation (89) by the product of a longitudinal wave function and the Landau wavefunction for motion in the uniform magnetic field $\beta = B\cos\theta$ similar to equation (75)

$$\psi_{k,m}(z, y) = \psi_k(z)\psi_m(y - y_0), \tag{106}$$

$$\psi_m(y) = (\frac{\beta}{\pi})^{1/4} \frac{1}{\sqrt{2^m m!}} H_m(\sqrt{\beta}y) \exp(-\frac{\beta}{2}y^2). \tag{107}$$

Here $H_m(y)$ are the Hermite polynomials and y_0 is the coordinate of the stable periodic orbit in the center of the stable island (it is assumed that this orbit is perpendicular to the first wall.) The energy of such states are exactly the same as before and in this approximation the tunneling current associated with such a stable island can be approximated by

$$\Gamma = 2\pi \sum_{N,m} |W_m|^2 \delta(E - E_{N,m}), \tag{108}$$

where $E_{N,m}$ are defined by equation (105) and the W_m are the integrals of overlap of the initial wavefunction as in (75) with $\psi_m(y)$ given by equation (107). In [15] it is shown that this description is in reasonable agreement with the results of numerical computation.

The purpose of this section is to demonstrate that the expansion of our expression for the tunneling current in powers of $e^{in\phi}$ and the summation of the resulting series on n, in the spirit of the Miller transformation of the Gutzwiller trace formula, leads to the above-discussed picture of separable motion in the vicinity of a stable periodic orbits. The final formula generalizes the one from reference [15] as it includes the wave functions connected with the exact Hamiltonian for the perpendicular motion and depends on exact monodromy matrix elements and not the approximate ones given by equation (107) which depend on the universal value $\beta = B\cos\theta$. The latter approximation is valid only for small θ.

According to equations (97, 98, 99) the tunneling current is

$$\Gamma = \frac{1}{2}\Gamma_p \sum_{r=1}^{\infty} D(r)^{-1/2} \exp(\mathrm{i}r(S_p - \frac{\pi}{2}\mu_p) + \mathrm{i}\Delta S(r)) + \text{c.c.}, \tag{109}$$

where S_p and μ_p are the action and Maslov index for the periodic orbit considered. The prefactor $D(r)$ and the exponent $\Delta S(r)$ are expressed through the monodromy matrix elements by the following expressions

$$D(r) = m_{21}^{(r)} + \mathrm{i}\beta\left(m_{11}^{(r)} + m_{22}^{(r)}\right) - \beta^2 m_{12}^{(r)}, \tag{110}$$

and

$$\Delta S(r) = \frac{\mathrm{i}\beta^2}{2D(r)}[y_0^2(m_{22}^{(r)} + \mathrm{i}\beta m_{12}^{(r)}) + y_0'^2(m_{11}^{(r)} + \mathrm{i}\beta m_{12}^{(r)}) + 2y_0y_0']. \tag{111}$$

The $m_{ij}^{(r)}$ are the monodromy matrix elements of the rth repetition of the primitive periodic orbit. Their dependence on r is given in equation (63). Let us consider in detail the case of a self-retracing stable where $m_{11} = m_{22}$ and $\lambda = \mathrm{e}^{\mathrm{i}\phi}$. In such a case

$$M^r = \begin{pmatrix} \cos\phi r & \rho\sin\phi r \\ -\rho^{-1}\sin\phi r & \cos\phi r \end{pmatrix}, \tag{112}$$

where

$$\rho = \frac{m_{12}}{\sin\phi}\cdot$$

Substituting these values into (110) and (111) one obtains

$$D(r) = -(1/\rho + \beta^2\rho)\sin\phi r + 2\mathrm{i}\beta\cos\phi r = \mathrm{i}\frac{\mathrm{e}^{\mathrm{i}\phi r}}{2\rho}[1 + \beta\rho]^2[1 - z^2], \tag{113}$$

where

$$z=\frac{\beta\rho-1}{\beta\rho+1}\mathrm{e}^{-\mathrm{i}\phi r},$$

and

$$\Delta S(r)=\frac{\mathrm{i}\beta^2}{2D(r)}((\cos\phi r+\mathrm{i}\beta\rho\sin\phi r)(y_0^2+y_0'^2)+2y_0y_0') \\ =\frac{\beta^2\rho(y_0^2+y_0'^2)}{2(1+\beta\rho)}-\frac{\beta^2\rho((y_0^2+y_0'^2)z^2-2y_0y_0'z)}{(\beta^2\rho^2-1)(1-z^2)}. \tag{114}$$

In order to expand the resulting expression and obtain a series in powers of $\exp(-\mathrm{i}\phi r)$ we shall use the following identity [26]

$$\frac{1}{\sqrt{1-z^2}}\exp\left(-\frac{(x^2+y^2)z^2-2xyz}{1-z^2}\right)= \\ \sum_{n=0}^{\infty}\frac{z^n}{2^n n!}H_n(x)H_n(y). \tag{115}$$

Finally

$$\Gamma=\frac{\Gamma_p\sqrt{\rho}}{(1+\beta\rho)\sqrt{2}}\exp\left(-\frac{\beta^2\rho}{2(1+\beta\rho)}(y_0^2+y_0'^2)\right) \\ \times\sum_{n=0}^{\infty}\frac{1}{2^n n!}H_n(\lambda y_0)H_n(\lambda y_0')\left(\frac{\beta\rho-1}{\beta\rho+1}\right)^n\sum_{r=-\infty}^{\infty}\mathrm{e}^{\mathrm{i}\Phi_n r} \tag{116}$$

where

$$\lambda=\frac{\beta\sqrt{\rho}}{\sqrt{\beta^2\rho^2-1}}$$

and

$$\Phi_n=S_p-\pi/2\mu_p-\phi(n+1/2).$$

But the sum $\sum_r\exp(\mathrm{i}\Phi_p r)$ is the same as the one considered above in equation (103) and it will give the sum over the δ-functions of the energy levels E_n defined by equation (105) and

$$\Gamma=\frac{\pi(\beta\rho)^{1/2}}{1+\beta\rho}\frac{\Gamma_1}{T}\exp\left(-\frac{\beta}{2(1+\beta\rho)}(y_0^2+y_0'^2)\right) \\ \times\left|(1-r_1)\sqrt{\frac{k}{k_z}}+(1+r_1)\sqrt{\frac{k_z}{k}}\right|^2 \\ \times\sum_{n=0}^{\infty}\frac{1}{2^n n!}H_n(\lambda y_0)H_n(\lambda y_0')\left(\frac{\beta\rho-1}{\beta\rho+1}\right)^n \\ \times\sum_N\delta(E-E_{N,n}). \tag{117}$$

To find an interpretation of this result one has to consider in more details the Hamiltonian for the motion perpendicular to the trajectory. The explicit form of this Hamiltonian can be found by different methods. The most straightforward one consists of the calculation first of the action $S(y,y')$ for r rotations in the vicinity of a given primitive periodic trajectory. As above

$$S_r(y,y')=\frac{1}{2}\left(\frac{\partial^2 S}{\partial y^2}y^2+2\frac{\partial^2 S}{\partial y\partial y'}yy'+\frac{\partial^2 S}{\partial y'^2}y'^2\right) \\ =\frac{m_{11}^{(r)}y^2+m_{22}^{(r)}y'^2-2yy'}{2m_{12}^{(r)}}. \tag{118}$$

Using equation (112) one can express $m_{ij}^{(r)}$ through $\mathrm{e}^{\pm\mathrm{i}r\phi}$

$$M^r=\begin{pmatrix}\cos\phi r+\rho\gamma\sin\phi r & \rho\sin\phi r\\ -(\rho^{-1}+\gamma^2\rho)\sin\phi r & \cos\phi r-\rho\gamma\sin\phi r\end{pmatrix}, \tag{119}$$

where

$$\rho=\frac{m_{12}}{\sin\phi}$$

and

$$\gamma=\frac{m_{11}-m_{22}}{2m_{12}}.$$

Putting formally $r\phi=\omega t$ where $\omega=\phi/T_p$ one gets the expression for $S(y,y';t)$. Now the Hamiltonian $H(p,y)$ can be obtained from the standard relation

$$H=\frac{\partial S}{\partial t}$$

by expressing in this result the coordinate y' of the first point through the initial momentum p, $p=-\partial S/\partial y$. In this way one obtains

$$H(p,y)=\frac{\omega}{2}\left(\rho(p+\gamma y)^2+\frac{1}{\rho}y^2\right). \tag{120}$$

It is easy to see that the monodromy matrix for this Hamiltonian for the time $t=T_p$ leads to equation (119) as it should be. It is this Hamiltonian which describes motion in the direction perpendicular to the trajectory.

We shall restrict ourselves to self-retracing orbits for which $m_{11}=m_{22}$ which is consistent with the fact that only orbits with $p_y=0$ at the LH wall will contribute appreciably. The other orbits contributions are semiclassically small. In such a case the quantum Hamiltonian in the perpendicular coordinate is

$$H(p,y)=\frac{\omega}{2}\left(\rho p^2+\frac{1}{\rho}y^2\right). \tag{121}$$

Its normalized eigenfunctions $\phi_n(y)$ are easily expressed through the Hermite polynomials[2]

$$\phi_n(y)=\frac{1}{(\pi\rho)^{1/4}}\frac{1}{\sqrt{2^n n!}}\exp\left(-\frac{y^2}{2\rho}\right)H_n\left(\frac{y}{\sqrt{\rho}}\right). \tag{122}$$

[2] Eigenfunctions of the Hamiltonian (120) with $\gamma\neq 0$ take the product form, $\exp(-\mathrm{i}\gamma y^2/2)\phi_n(y)$.

This function corresponds to the energy $E_n = \omega(n+1/2)$. Note that the $\phi_n(y)$ depend explicitly on points of the trajectory because $\rho = m_{12}/\sin\theta$ changes along the trajectory. On the other hand the energy of the perpendicular motion depends only on $\omega = \phi/T_p$ which is a canonical invariant and stays the same at any point on the trajectory considered.

Therefore the wave function in the vicinity of a stable orbit can be written as a product of longitudinal and perpendicular wave functions as in equation (106) but with $\psi_m(y)$ replaced by $\phi_m(y)$ from (122) and the normalized longitudinal wave $\psi_k(z)$ chosen in the following WKB form

$$\psi_k(z) = \frac{A}{\sqrt{k(z)}}\cos(\int_0^z k(z')\mathrm{d}z' + \phi/2). \tag{123}$$

Here $k(z)$ is the momentum in the z direction, ϕ is the reflection phase, $r_1 = \exp(\mathrm{i}\phi)$, and the normalization constant $|A|^2 = 4/T$ where T is the primitive classical period of motion

$$T = \oint \frac{\mathrm{d}z}{k(z)}\cdot$$

The overlap integral (89) becomes

$$\begin{aligned} W_m(y_0) &= \frac{A}{2\sqrt{k}}(k_z\cos(\phi/2) + \mathrm{i}k\sin(\phi/2)) \\ &\quad\times\int \psi_0(y,0)\phi_m(y-y_0)\mathrm{d}y \\ &= \Lambda_m\int\exp\left(-\frac{\beta y^2}{2} - \frac{(y-y_0)^2}{2\rho}\right)H_m\left(\frac{y-y_0}{\sqrt{\rho}}\right)\mathrm{d}y, \end{aligned} \tag{124}$$

where

$$\begin{aligned} \Lambda_m &= \frac{AC}{2(2^m\pi m!)^{1/2}}\left(\frac{\beta}{\rho}\right)^{1/4} \\ &\quad\times\left(\sqrt{\frac{k_z}{k}}\cos(\phi/2) + i\sqrt{\frac{k}{k_z}}\sin(\phi/2)\right). \end{aligned} \tag{125}$$

In deriving these expressions it was taken into account that the z-component of the momentum in the QW is approximately equal to the total momentum k. The constant C and the momentum k_z come from the initial wave function (27).

This integral can be easily computed using the relation from [26]

$$\begin{aligned} &\frac{1}{\sqrt{2\pi u}}\int_{-\infty}^{\infty}\mathrm{d}u\ H_n(u)\mathrm{e}^{-\frac{(x-u)^2}{2u}} = \\ &\qquad\sqrt{(1-2u)^n}H_n\left(\frac{x}{\sqrt{1-2u}}\right). \end{aligned} \tag{126}$$

One obtains

$$\begin{aligned} W_m &= \Lambda_m\sqrt{\frac{2\pi\rho}{1+\beta\rho}} \\ &\quad\times\exp\left(-\frac{\beta y_0^2}{2(1+\beta\rho)}\right)\left(\frac{\beta\rho-1}{\beta\rho+1}\right)^{m/2}H_m(-\lambda y_0), \end{aligned} \tag{127}$$

where

$$\lambda = \frac{\beta\sqrt{\rho}}{\sqrt{(\beta\rho)^2-1}}\cdot$$

Performing the summation one finds

$$\begin{aligned} \Gamma &= \frac{4\pi(\beta\rho)^{1/2}}{1+\beta\rho}\frac{\Gamma_1}{T}\exp\left(-\frac{\beta}{2(1+\beta\rho)}(y_0^2+y_0'^2)\right) \\ &\quad\times\left(\frac{k_z}{k}\cos^2(\phi/2) + \frac{k}{k_z}\sin^2(\phi/2)\right) \\ &\quad\times\sum_m\frac{1}{2^m m!}\left(\frac{\beta\rho-1}{\beta\rho+1}\right)^m H_m(\lambda y_0)H_m(\lambda y_0') \\ &\quad\times\sum_N\delta(E-E_{N,m}), \end{aligned} \tag{128}$$

where $E_{N,m}$ are defined in equation (105). As

$$\begin{aligned} &\left|(1-r_1)\sqrt{\frac{k}{k_z}} + (1+r_1)\sqrt{\frac{k_z}{k}}\right|^2 = \\ &\qquad 4\left(\frac{k_z}{k}\cos^2(\phi/2) + \frac{k}{k_z}\sin^2(\phi/2)\right), \end{aligned}$$

this result exactly coincides with the Miller type expansion of our semiclassical formula given by equations (117).

10 Conclusion

We have developed a semiclassical theory of resonant tunneling from a quasi-bound state which enters a QW and tunnels through a second barrier at the other end of the QW. The final result is a series of semiclassical expressions for the tunneling current of electrons arriving at the second interface. The first formula (Eq. (66)) applies to the ergodic regime and gives the contribution of strongly unstable periodic orbits. In this regime standard semiclassical arguments proved that a good approximation can be achieved by expanding the actions up to quadratic terms and performing the integration by the saddle point method. The second case (Eqs. (87, 99)) corresponds to stable or slightly unstable orbits and is really a generalization of the first one. In this case one should base on the assumption that the dynamics in the neighborhood of such orbits is controlled by a one-dimensional quadratic potential so that the actions in perpendicular coordinates are still close to being quadratic and, consequently, can easily be integrated exactly. For big stable regions the Miller-type formula (see Eq. (117)) is appropriate.

Our calculation demonstrated that in the semiclassical approximation the tunneling current is due to special periodic orbits which in order to contribute significantly should obey the following two conditions:

- hit the RH wall and
- be perpendicular to the LH wall.

The contribution of such periodic orbits to the tunneling current has a form similar to the Gutzwiller trace formula for the density of state but for (strongly unstable orbits) it is proportional to the $(m_{21})^{-1/2}$ matrix element.

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Appendix A: Perturbation theory of tunneling probability

The purpose of this appendix is to show that equation (31), which expresses the wave function inside the quantum well through boundary values of the wave function of the bound state in the emitter, can be interpreted as the result of first order perturbation theory on the tunneling amplitude quite similar to the one used by Bardeen [17].

Let us assume that there exist two wells separated by a barrier between points z_a and z_b and let $\Phi_0(\mathbf{x})$ be a wavefunction of a bound state in the first well which would exist if the second well were absent.

Analogously let us introduce the wavefunctions $\psi_n(\mathbf{x})$ which are the wavefunctions of the bound states in the second well under the assumption that the first well is absent.

Both $\Phi_0(\mathbf{x})$ and $\psi_n(\mathbf{x})$ are not the true eigenfunctions of our Hamiltonian, $\hat{H}$, but of two new Hamiltonians $\hat{H}_{\rm L}$ and $\hat{H}_{\rm R}$

$$\hat{H}_{\rm L}\Phi_0 = E_0\Phi_0, \quad \hat{H}_{\rm R}\psi_n = E_n\psi_n, \tag{A.1}$$

which differ from $\hat{H}$

$$\hat{H}_{\rm L} = \hat{H} - V_{\rm L}, \quad \hat{H}_{\rm R} = \hat{H} - V_{\rm R}, \tag{A.2}$$

by certain potentials $V_{\rm L}$ and $V_{\rm R}$ which by construction equal zero in the following intervals

$$\begin{aligned} V_{\rm L}(\mathbf{x}) = 0 \quad &\text{if} \quad z < z_b, \\ V_{\rm R}(\mathbf{x}) = 0 \quad &\text{if} \quad z > z_a. \end{aligned} \tag{A.3}$$

Note that both $\Phi(\mathbf{x})$ and $\psi_n(\mathbf{x})$ are eigenfunctions of $\hat{H}$ inside the barrier. Now it is natural to use perturbation theory on $V_{\rm L}$ (or $V_{\rm R}$) corresponding to the representation (A.2) as the sum of two terms. The main difficulty here comes from the fact that the perturbation $V_{\rm L,R}$ cannot be considered as a small one because it produces bound states. It is known [27] that in such a situation the usual perturbation theory diverges and it is necessary to incorporate all bound states on equal footing.

Therefore we shall look for the exact wavefunctions of the Hamiltonian $\hat{H} = \hat{H}_{\rm L} + V_{\rm L}$ as a sum over all unperturbed states

$$\psi(\mathbf{x}) = c_0\phi_0(\mathbf{x}) + \sum_n b_n\psi_n(\mathbf{x}), \tag{A.4}$$

and the corresponding expansion of the energy of this state.

In the zeroth order $c_0 = 1$ and $b_n = 0$. In the next order one has to take into account the matrix elements of the transition matrix between Φ_0 and ψ_n,

$$V_{n0} = \langle\psi_n|V_l|\Phi_0\rangle.$$

Standard formulae for the first terms of perturbation theory (see *e.g.* [19]) give

$$\begin{aligned} b_n^{(1)} &= \frac{1}{E_0 - E_n}V_{n0}, \\ E &= E_0 + \langle\Phi_0|V_{\rm L}|\Phi_0\rangle + \sum_n \frac{|V_{n0}|^2}{E_0 - E_n}\cdot \end{aligned} \tag{A.5}$$

For the computation V_{n0} we follow (with modifications) the method of Bardeen in reference [17]

$$\begin{aligned} V_{n0} &= \int {\rm d}\mathbf{x}\bar{\psi}_n(\mathbf{x})V_{\rm L}(\mathbf{x})\Phi_0(\mathbf{x}){\rm d}\mathbf{x} \\ &= \int_{z_b}^{\infty} {\rm d}\mathbf{x}\bar{\psi}_n(\hat{H} - E_0)\Phi_0, \end{aligned} \tag{A.6}$$

where we put the limits of the integration on the z variable in order to stress that outside this region the integral is zero. Using the fact that

$$(\hat{H} - E_n)\psi_n = 0$$

when $x > x_a$ the integrand in the precedent equation can be rewritten in the more symmetric form

$$V_{n0} = \int_{z_b}^{\infty} \Big(\bar{\psi}_n\hat{H}\Phi_n - \hat{H}\bar{\psi}_n\Phi_0 + (E_n - E_0)\bar{\psi}_n\Phi_0\Big). \tag{A.7}$$

As the most important states are the ones for which $E_n \approx E_0$ one can neglect the second term in this expression and

$$V_{n0} = \int_{z_b}^{\infty} \Big(\bar{\psi}_n\hat{H}\Phi_n - \hat{H}\bar{\psi}_n\Phi_0\Big)\,{\rm d}\mathbf{x}. \tag{A.8}$$

As

$$\hat{H} = -\frac{1}{2m}\triangle + V(\mathbf{x}),$$

the integrand in this expression is the divergence of the current

$$\bar{\psi}_n \hat{H}\Phi_0 - \hat{H}\bar{\psi}_n\Phi_0 = -\frac{1}{2m}\nabla_\mu\left(\bar{\psi}_n\nabla_\mu\Phi_0 - \nabla_\mu\bar{\psi}_n\Phi_0\right). \quad (A.9)$$

Performing the integration in equation (A.8) and taking into account that the boundary terms at infinity vanish one concludes that

$$V_{n0} = \frac{1}{2m}\int \mathrm{d}\mathbf{q}\left(\bar{\psi}(\mathbf{q})\frac{\partial}{\partial z}\Phi_0(\mathbf{q}) - \frac{\partial}{\partial z}\bar{\psi}_n(\mathbf{q})\Phi(\mathbf{q})\right), \quad (A.10)$$

where $\mathbf{q} = (y, z_b)$ is the vector on the wall of the barrier at $z = z_b$ and the integral is taken over the whole left-hand wall of the second well. Using equation (A.4, A.5, A.10) we obtain that the wavefunction in the second well has the form (note that $\Phi_0(\mathbf{x})$ is exponentially small in this region)

$$\begin{aligned}\psi(\mathbf{x}) &= \frac{1}{2m}\sum_n \frac{1}{E_0 - E_n}\psi_n(\mathbf{x}) \\ &\times \int \mathrm{d}\mathbf{q}\left(\bar{\psi}_n(\mathbf{q})\frac{\partial}{\partial z}\Phi_0(\mathbf{q}) - \frac{\partial}{\partial z}\bar{\psi}_n(\mathbf{q})\Phi_0(\mathbf{q})\right) \\ &= \frac{1}{2m}\int \mathrm{d}\mathbf{q}\left(\frac{\partial\Phi_0(\mathbf{q})}{\partial z}G(\mathbf{x},\mathbf{q};E) - \frac{\partial G(\mathbf{x},\mathbf{q};E)}{\partial z}\Phi_0(\mathbf{q})\right),\end{aligned} \quad (A.11)$$

where we have introduced the Green function for the motion in the second well as in equation (90).

This expression exactly coincides with equation (33) derived from the semiclassical matching procedure described in Section 5.The same formalism permits us also to compute the imaginary part of the energy level in (A.5). Putting $E = E + \mathrm{i}\epsilon$ and $\epsilon \to 0$ one gets that $E = E - \mathrm{i}\Gamma/2$ where

$$\Gamma = 2\pi\sum_n |V_{n0}|^2\delta(E_0 - E_n). \quad (A.12)$$

This is the Fermi Golden rule which using (A.10) reproduces the Bardeen result in [17].

Appendix B: Resonant tunneling in one dimension

In this appendix we shall discuss the calculation of the tunneling current through a one dimensional resonant diode. Our main purpose here is to clarify the above-discussed method on a soluble example.

Let us consider a one step-wise barrier. Wave function before the barrier has the form of a sum of two exponents

$$\psi(z) = \frac{1}{\sqrt{k_1}}(a\exp(\mathrm{i}k_1 z) + b\exp(-\mathrm{i}k_1 z)), \quad (B.1)$$

and after the barrier it has the same form but with different coefficients a' and b'

$$\psi(z) = \frac{1}{\sqrt{k_2}}(a'\exp(\mathrm{i}k_2 z) + b'\exp(-\mathrm{i}k_2 z)). \quad (B.2)$$

Here k_1 and k_2 are the momentum in the corresponding regions.

Coefficients a, b and a', b' are connected by a transfer matrix whose general form follows from the current conservation

$$\begin{pmatrix} a' \\ b' \end{pmatrix} = \begin{pmatrix} \alpha & \beta \\ \bar{\alpha} & \bar{\beta} \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix}, \quad (B.3)$$

with $|\alpha|^2 - |\beta|^2 = 1$.

The reflection r_l, and transmission, t_l, coefficients for the motion from left to right are defined by the condition that after the barrier there is no in-coming wave

$$t_\mathrm{l} = \frac{1}{\bar{\alpha}}, \quad r_\mathrm{l} = -\frac{\bar{\beta}}{\bar{\alpha}}\cdot \quad (B.4)$$

The same quantities but for the motion from right to left have the following values

$$t_\mathrm{r} = \frac{1}{\bar{\alpha}}, \quad r_\mathrm{r} = \frac{\beta}{\bar{\alpha}}\cdot \quad (B.5)$$

Of course, in any case $|r|^2 + |t|^2 = 1$.

Now let we have two barriers separated by a quantum well of the width L and with momentum k. The total transfer matrix is the product of three matrices corresponding respectively to the tunneling through the first barrier (parameters α_1 and β_1), free motion through the quantum well (parameters k and L), and the tunneling through the second barrier (parameters α_2 and β_2):

$$\begin{pmatrix} \alpha_{12} & \beta_{12} \\ \bar{\alpha}_{12} & \bar{\beta}_{12} \end{pmatrix} = \begin{pmatrix} \alpha_2 & \beta_2 \\ \bar{\alpha}_2 & \bar{\beta}_2 \end{pmatrix}\begin{pmatrix} \exp(\mathrm{i}kL) & 0 \\ 0 & \exp(-\mathrm{i}kL) \end{pmatrix}\begin{pmatrix} \alpha_1 & \beta_1 \\ \bar{\alpha}_1 & \bar{\beta}_1 \end{pmatrix}\cdot \quad (B.6)$$

From this relation one finds

$$\begin{aligned}\alpha_{12} &= \alpha_1\alpha_2\exp(\mathrm{i}kL) + \bar{\beta}_1\beta_2\exp(-\mathrm{i}kL) \\ \beta_{12} &= \beta_1\alpha_2\exp(\mathrm{i}kL) + \bar{\alpha}_1\beta_2\exp(-\mathrm{i}kL).\end{aligned} \quad (B.7)$$

The total transmission coefficient through this resonant diode, $t_{12} = 1/\bar{\alpha}_{12}$, equals

$$\begin{aligned}t_{12} &= \frac{1}{\bar{\alpha}_1\bar{\alpha}_2\exp(-\mathrm{i}kL) + \beta_1\bar{\beta}_2\exp(\mathrm{i}kL)} \\ &= t_1\exp(\mathrm{i}kL)\sum_{n=0}^{\infty}(R\exp(2\mathrm{i}kL))^n t_2,\end{aligned} \quad (B.8)$$

Here $R = r_1 r_2$ and r_1, t_1 and r_2, t_2 are the reflection and transmission coefficients through the left and right barrier respectively (see (B.4, B.5)).

This formula has the clear physical meaning. The total transmission amplitude is constructed by a few simple steps. First of all, the particle has to tunnel into the quantum well (the amplitude of which is described by t_1), then it has to propagate to the second barrier (factor $\exp(\mathrm{i}kL)$), then it can perform an arbitrary number, n, of loops inside the quantum well (the contribution of each loop equals $r_1 r_2 \exp(2\mathrm{i}kL)$) before it can tunnel through the second wall with amplitude t_2.

By adjusting this two-barrier structure to a "emitter" well one can calculate the imaginary part of a quasi-bound state formed at the emitter by the standard formula (which is the lowest order of perturbation theory of tunneling probability)

$$\Gamma = \frac{1}{T}|t_{12}|^2, \tag{B.9}$$

where T is the period of motion in the emitter well. The first factor here, $1/T$, is the number of collisions with the wall per unit time and every time the particle hits the wall it has a probability of tunneling through it equal $|t_{12}|^2$. Here only the possibilities of tunneling back to the emitter are neglected.

Substituting here equation (B.8) one gets

$$\begin{aligned}\Gamma &= \frac{1}{T|\bar{\alpha}_1\bar{\alpha}_2\exp(-\mathrm{i}kL)+\beta_1\bar{\beta}_2\exp(\mathrm{i}kL)|^2}\\ &= \frac{|t_1|^2}{T}|t_2|^2|\sum_{n=0}^{\infty}(R\exp(2\mathrm{i}kL))^n|^2.\end{aligned} \tag{B.10}$$

The first factor here is the imaginary part of the quasi-bound state at the emitter without the second barrier which we called Γ_1. The double sum over n and m

$$|\sum_{n=0}^{\infty}(R\exp(2\mathrm{i}kL))^n|^2 = \sum_{n,m=0}^{\infty} R^n\bar{R}^m\exp(2\mathrm{i}kL(n-m)) \tag{B.11}$$

can be computed by substitution $r = n - m$. The final result is the following

$$\Gamma = \Gamma_1\frac{|t_2|^2}{1-|R|^2}\left(1+\sum_{r=1}^{\infty}R^r\exp(\mathrm{i}Sr)+\mathrm{c.c.}\right), \tag{B.12}$$

where $S = 2kL$ is the classical action inside the quantum well. This formula is an analog of equation (66) but for one-dimensional case. We stress that this is an exact result for the one-dimensional problem considered and no approximation except ones leading to equation (B.9) has been made.

Now we shall obtain the same result first by using the Green function method as was done above and second by using directly the current conservation. The advantage of the former is extreme physical clarity of calculation. One just follows the particle and computes corresponding factors for each possible process. From mathematical point of view this method corresponds to the time evolution of wave packet initially localized in the emitter well. The second method is more formal and corresponds to a stationary picture of tunneling. The both will lead to the same answer which coincides with equation (B.12).

To compute the tunneling probability we have to know the total in-coming current in a vicinity of the second barrier. The corresponding wave function is given by the same expression as in equation (33) but, evidently, without the integration over perpendicular coordinate

$$\psi(z) = \frac{1}{2m}(G(z,z')\partial_{z'}\psi_1(z') - \partial_{z'}G(z,z')\psi(z'))|_{z'=0}. \tag{B.13}$$

Here $\psi_1(z')$ is the wave function just after the tunneling point and $G(z,z')$ is the Green function for the motion from point z' to point $z > z'$ inside the well which can be written in the form

$$\begin{aligned}G(z,z') = \frac{m}{\mathrm{i}k}(&\exp(\mathrm{i}k(z-z'))\\ &+ r_1\exp(\mathrm{i}k(z+z'))\left(\sum_{n=0}^{\infty}(r_1r_2)^n\exp(2\mathrm{i}kLn)\right).\end{aligned} \tag{B.14}$$

The first term is just the free Green function. The second one corresponds to the trajectory first reflected from the left boundary and then passing through the final point. Of course, its contribution should be multiplied by the reflection coefficient from the first wall, r_1. The sum in the second bracket corresponds to trajectories which perform an arbitrary number of full loops, n, before coming to the end point. The contribution of each loop includes the usual phase factor $\exp(2\mathrm{i}kL)$ and also reflection coefficients from both walls.

Similar to equation (25)

$$\psi_1(z) = \frac{C}{\sqrt{k}}\exp(\mathrm{i}kz), \tag{B.15}$$

where $|C|^2 = m\Gamma_1$ and by calculating the current in (B.13) we get

$$\psi(z) = \frac{C}{\sqrt{k}}\exp(\mathrm{i}kz)\sum_{n=0}^{\infty}(r_1r_2)^n\exp(2\mathrm{i}kLn). \tag{B.16}$$

Note that the result do not depend on the reflection coefficient in front of the second term in (B.14) as it should be from physical considerations and effectively only one trajectory gives the contribution.

The total imaginary part of the quasi-bound state in the emitter well is given by the same formula as equation (8) in [1] (without the integration)

$$\Gamma = j|t_2|^2, \tag{B.17}$$

where j is the in-coming current at the second wall

$$j = \frac{1}{2\mathrm{i}m}(\bar{\psi}(z)\partial_z\psi(z) - \psi(z)\partial_z\bar{\psi}(z))|_{z=L}. \tag{B.18}$$

Finally one obtains

$$\Gamma = \Gamma_1|\sum_{n=0}^{\infty}(r_1r_2)^n\exp(2\mathrm{i}kLn)|^2, \tag{B.19}$$

which is the same as in equation (B.12). Therefore the Green function method gives the exact answer for one-dimensional tunneling.

In the second method there is no need to separate only one part of the full current as it was done in equation (B.14) (though it leads to very clear picture of the process). One can instead compute the total current anywhere inside the quantum well. In this case it is necessary to know the full Green function inside the quantum well. Contrary to equation (B.14) it will include four terms

$$\begin{aligned} G(z,z') = \frac{m}{\mathrm{i}k}&(\exp(\mathrm{i}k(z-z')) + r_1\exp(\mathrm{i}k(z+z') \\ &+ r_2\exp(\mathrm{i}k(2L-z-z') \\ &+ r_1r_2\exp(\mathrm{i}k(2L-z+z')) \\ &\times\left(\sum_{n=0}^{\infty}(r_1r_2)^n\exp(2\mathrm{i}kLn)\right). \end{aligned} \quad \text{(B.20)}$$

The third term in this expression corresponds to a trajectory which is reflected from the second wall before coming to final point and the forth one appears from a trajectory which first hits the left wall then reflected from the right wall and only after this motion return to final point. As usual each type of trajectories can be accompanied by an arbitrary number of full rotations. It is this Green function which obeys all boundary conditions.

By computing the current in equation (B.18) one gets

$$\begin{aligned} \psi(z) = \frac{C}{\sqrt{k}}&(\exp(\mathrm{i}kz) + r_2\exp(\mathrm{i}k(2L-z)) \\ &\times\left(\sum_{n=0}^{\infty}(r_1r_2)^n\exp(2\mathrm{i}kLn)\right). \end{aligned} \quad \text{(B.21)}$$

As above only trajectory corresponding to out-going current from the left wall give non-zero contribution. The total imaginary part is equal to the total current (B.18) but now there is no necessity to compute it at $z = L$ as the current is independent on z.

Simple computation gives

$$\Gamma = \Gamma_1(1-|r_2|^2)|\sum_{n=0}^{\infty}(r_1r_2)^n\exp(2\mathrm{i}kLn)|^2. \quad \text{(B.22)}$$

As $1-|r_2|^2 = |t_2|^2$ this answer coincides with the result above.

When the tunneling through the second barrier is much bigger than through the first one the dependence on t_2 will disappear because in this case $r_1 \approx 1$, $1-|R|^2 = |t_2|^2$, and the ratio $|t_2|^2/(1-|R|^2)$ in above expressions tends to 1 as it should be.

References

1. R. Balian, C. Bloch, Ann. Phys. NY **69**, 76 (1972).
2. M. Gutzwiller, *Chaos in Classical and Quantum Mechanics* (Springer-Verlag, New York, 1990).
3. M. Berry, Lect. Notes Phys. **263**, 1 (1986).
4. Les Houches Summer School, 1989, *Chaos and Quantum Physics*, edited by M.J. Giannoni, A. Voros, J. Zinn-Justin (Elsevier, New York, 1991).
5. E. Heller in [4].
6. P.B. Wilkinson, T.M. Fromhold, L. Eaves, F.W. Sheard, N. Miura, T. Takamasu, Nature **380**, 6575 (1997).
7. H. Friedrich, D. Wintgen, Phys. Rep. **183**, 37 (1989).
8. E. Bogomolny, Sov. Phys. JETP **69**, 275 (1989).
9. H.U. Baranger, R.A. Jalabert, A.D. Stone, Phys. Rev. Lett. **70**, 3876 (1993).
10. T.M. Fromhold, P.B. Wilkinson, F.W. Sheard, L. Eaves, J. Miao, G. Edwards, Phys. Rev. Lett. **75**, 1142 (1995).
11. G. Müller, G.S. Boebinger, H. Mathur, L.N. Pfeiffer, K.W. West, Phys. Rev. Lett. **75**, 2875 (1995).
12. D.L. Shepelyansky, A.D. Stone, Phys. Rev. Lett. **74**, 2098 (1974).
13. T.S. Monteiro, P.A. Dando, Phys. Rev. E **53**, 3369 (1996).
14. T.S. Monteiro, D. Delande, A.J. Fisher, G.S. Boebinger, Phys. Rev. E **56**, 3913 (1997).
15. T.S. Monteiro, D. Saraga, Phys. Rev. E **57**, 5252 (1998).
16. E. Bogomolny, D. Rouben, Europhys. Lett. **43**, 111 (1998).
17. J. Bardeen, Phys. Rev. Lett. **6**, 57 (1966).
18. M.L. Leadbeater, F.W. Sheard, L. Eaves, Semicon. Sci. Technol. **6**, 1021 (1991).
19. L.D. Landau, E.M. Lifshitz, *Quantum Mechanics* (Butterworth-Heinemann, Linacre House, Oxford, 1997).
20. E. Bogomolny, Physica D **31**, 169 (1988).
21. S.C. Creagh, J.M. Robbins, R.G. Littlejohn, Phys. Rev. A **42**, 1907 (1990).
22. K. Richter, D. Ullmo, R.-A. Jalabert, Phys. Rep. **276**, 1 (1996).
23. P. Gaspard, D. Allonso, Phys. Rev. A **47**, R3468 (1993).
24. R.P. Feymann, A.R. Hibbs, *Quantum mechanics and Path Integrals* (McGraw-Hill Publishing Company, 1965).
25. W. Miller, J. Chem. Phys. **63**, 996 (1975).
26. *Higher Transcendental Functions*, edited by A. Erdélyi (McGraw-Hill Publishing Company, 1953), Vol. II, p. 195.
27. R.G. Newton, *Scattering Theory of Waves and Particles* (McGraw-Hill Publishing Company, 1966).