Path-integral approach to resonant tunneling

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Resonant tunneling is studied by use of Feynman's path integrals. The semiclassical Green's function is obtained for a one-dimensional double-barrier structure. This approach leads to a clearer and deeper understanding of the physical process of resonant tunneling. It is shown that sequential tunneling never gives rise to negative differential resistance.

Resonant tunneling through double-barrier structures is one of the most interesting problems which attracts many theorists and experimentalists in the field of semiconductor physics. Since Chang, Esaki, and Tsu[1] first demonstrated negative differential resistance due to resonant tunneling in semiconductor heterostructures, a number of investigations have been devoted to this problem.[2-8] In spite of these efforts, the physics of resonant tunneling has not been sufficiently understood and some problems still remain matters of controversy. One such problem is whether the experimentally observed negative differential resistance is due to resonant tunneling or sequential tunneling proposed by Luryi.[2-4]

In this paper, we present Feynman's path-integral description of resonant tunneling. As is well known, the path-integral method[9,10] developed by Feynman is an alternative formulation for quantum mechanics and it has the advantage of pursuing the motion of electrons as if they were classical particles. Gutzwiller[11] has applied this method to the bound states of an atom. Freed[12] and McLaughlin[13] have independently extended the path-integral method capable of treating barrier tunneling by introducing an imaginary time. On the basis of these papers, we attempt to approach resonant tunneling by path integrals. The result obtained leads to a clearer and deeper understanding of resonant tunneling and also provides the foundation for further development.

In path-integral formulation, the semiclassical propagator from x' and x is written as[12]

$$K(x,t;x',0)=\sum_\alpha \left[\frac{1}{2\pi i\hbar}\frac{\partial^2 S(x,t;x',0)}{\partial x\,\partial x'}\right]^{1/2} \times \exp\left[\frac{i}{\hbar}S(x,t;x',0)-\tfrac{1}{2}(i\nu\pi)\right], \quad (1)$$

where

$$S(x,t;x',0)=\int_0^t d\tau \mathcal{L} ,$$

α labels the classical paths from $(x',0)$ to (x,t), ν is the number of times $\partial^2 S/\partial x\,\partial x'$ becomes infinite along the classical path, S is the Hamilton's principal function, and $\mathcal{L}$ is the classical Lagrangian for the system.

For electrons with definite energy E, it is convenient to use the Fourier transform of Eq. (1), the semiclassical Green's function,

$$G(x,x';E)=(i\hbar)^{-1}\int_0^\infty dt \exp\left[\frac{iEt}{\hbar}\right]K(x,t;x',0) . \quad (2)$$

After some calculations, we obtain

$$G(x,x';E)=(i\hbar)^{-1}\sum_\alpha \left|\frac{\partial^2 W(x,x';E)}{\partial E\,\partial x}\;\frac{\partial^2 W(x,x';E)}{\partial E\,\partial x'}\right|^{1/2} \times\exp\left[\frac{i}{\hbar}W(x,x';E)-\tfrac{1}{2}(i\nu\pi)\right], \quad (3)$$

where W is the classical action

$$W(x,x';E)=\int_{x'}^{x} p(x'';E)dx'' , \quad (4)$$

and p is the momentum. Freed[12] and McLaughlin[13] have independently extended Eq. (3) applicable to cases in which barrier tunneling occurs by taking time as an imaginary variable. According to them, Eq. (3) is still valid, but W, Eq. (4), is modified as

$$W(x,x';E)=\int_{x'}^{x} dx''\{2m[E-V(x'')]\}^{1/2} ,$$

where $V(x)$ ($>E$) is the barrier potential.

Now let us consider a one-dimensional double-barrier structure whose potential profile is shown in Fig. 1(a), where x_0, x_1, x_2, and x_3 are the potential turning points and V_0 is the barrier potential. For simplicity, we put $x_1-x_0=x_3-x_2=l$ and $x_2-x_1=L$.

We first consider the motion of electron incident from the left transmitted to the right. We denote this process as $x'\to x$, where we put $x'<x_0$ and $x_3<x$. The classical paths contributing to the transmission from x' to x, as shown in Fig. 1(b), are given as follows: t_0, direct motion from x' to x; t_1, $x'\to x_2\to x_1\to x_2\to x$ (one periodic path, $x_2\to x_1\to x_2$, is added to t_0); t_n, $x'\to n(x_2\to x_1\to x_2)\to x$ (n periodic paths are added to t_0). The components of the Green's function corresponding to the above paths can be written as follows: for t_0

$$g_0=\frac{m}{i\hbar\sqrt{p(x)p(x')}}\exp\left[\frac{i}{\hbar}\int_{x'}^{x_0}p(x'')dx''-\frac{1}{\hbar}\int_{x_0}^{x_1}q(x'')dx''+\frac{i}{\hbar}\int_{x_1}^{x_2}p(x'')dx''-\frac{1}{\hbar}\int_{x_2}^{x_3}q(x'')dx''+\frac{i}{\hbar}\int_{x_3}^{x}p(x'')dx''-i2\pi\right]$$

$$=\frac{1}{i\hbar}\left[\frac{m}{2E}\right]^{1/2}\exp\left[\frac{i}{\hbar}p[(x_0-x')+L+(x-x_3)]-2\kappa l\right], \quad (5)$$

for t_1

$$g_1=g_0[1-\exp(-2\kappa l)]\exp\left[\frac{i}{\hbar}\oint p\,dx''-i\pi\right], \quad (6)$$

and for t_n

$$g_n=g_0[1-\exp(-2\kappa l)]^n\exp\left[n\left[\frac{i}{\hbar}\oint p\,dx''-i\pi\right]\right], \quad (7)$$

where

$$p(x)=(2mE)^{1/2},$$

$$q(x)=[2m(V_0-E)]^{1/2}=\hbar\kappa,$$

$$\oint p\,dx''=2\int_{x_1}^{x_2}p\,dx''=2(2mE)^{1/2}L.$$

Here we introduce the factor $1-\exp(-2\kappa l)$ into Eqs. (6) and (7). For the present structure, when electrons are reflected from the barrier, a part of them tunnels through the barrier. As reflections take place twice during one periodic path, $x_2\rightarrow x_1\rightarrow x_2$, the probability amplitude reduces as $1-\exp(-2\kappa l)$. The semiclassical Green's function for transmission is then given as a sum over all the paths (t_n) for $n=0,1,\ldots,\infty$. We obtain

$$G(x,x';E)=\frac{1}{i\hbar}\left[\frac{m}{2E}\right]^{1/2}\times\exp\left[\frac{i}{\hbar}p[(x_0-x')+L+(x-x_3)]\right]Z_\infty(E), \quad (8)$$

where

$$Z_\infty(E)=\frac{\exp(-2\kappa l)}{1-[1-\exp(-2\kappa l)]\exp(i\phi)}, \quad (9)$$

$$\phi=\frac{1}{\hbar}\oint p\,dx''-\pi. \quad (10)$$

From the property of the Green's function, the transmission coefficient T is given as

$$T(E)=|Z_\infty(E)|^2.$$

When $\phi=2n\pi$ is satisfied, T becomes unity. All the trajectories interfere constructively and resonant tunneling occurs. Unless $\phi\simeq 2n\pi$ is satisfied (off resonance), the absolute value of the denominator of Eq. (9) is of the order of 1 and

$$T\propto\exp(-4\kappa l).$$

This means that individual trajectories interfere destructively. We can express the resonance condition as

$$\oint p\,dx''=(n+\tfrac{1}{2})h, \quad (11)$$

which is the well-known Bohr-Sommerfeld condition. Under this condition,

$$Z_\infty=\exp(-2\kappa l)\{1+[1-\exp(-2\kappa l)]+[1-\exp(-2\kappa l)]^2+[1-\exp(-2\kappa l)]^n+\cdots\}. \quad (12)$$

This equation represents how resonant tunneling develops with increasing the number of reflections. As described earlier, $1-\exp(-2\kappa l)$ indicates the reduction in the probability amplitude accompanying reflections. This term is characteristic of metastable states where electrons leak out from the potential well. On the contrary, electrons in bound states do not leak out, then the Green's

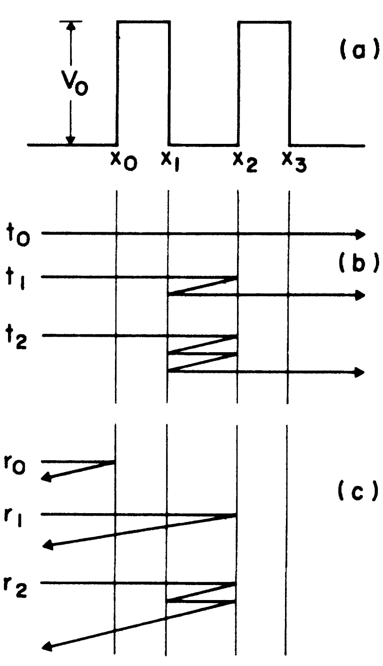

FIG. 1. (a) Energy-band diagram of a double-barrier structure, (b) semiclassical paths for transmission, and (c) semiclassical paths for reflection.

function of the system including bound states has poles in E plane.

In the above derivation of the Green's function, Eq. (8), we have assumed that electrons have an infinite lifetime and suffer no scattering during the traversals from x' to x. In a real case, however, scattering is unavoidable. Here we express the scattering effects by cutting off the number N of periodic motions of electrons in the well, in which case N is related to the scattering time τ in the well by

$$N+1 \simeq v\tau/(2L) , \tag{13}$$

using the electron velocity v given by

$$v=\sqrt{2E/m} . \tag{14}$$

Then $Z_\infty(E)$ of Eqs. (8) and (9) should be replaced by

$$\begin{aligned} Z_N(E) &= \exp(-2\kappa l)\{1+[1-\exp(-2\kappa l)]\exp(i\phi)+\cdots+[1-\exp(-2\kappa l)]^N\exp(iN\phi)\} \\ &= \frac{\exp(-2\kappa l)\{1-[1-\exp(-2\kappa l)]^{N+1}\exp[i(N+1)\phi]\}}{1-[1-\exp(-2\kappa l)]\exp(i\phi)} . \end{aligned} \tag{15}$$

This shows how the transmission varies with N. It can easily be seen from Eqs. (12) and (15) that, for $\exp(-2\kappa l) \ll 1$, as is often the case, N is a direct measure of enhancement of the transmission, that is, the transmission coefficient at resonance is $(N+1)^2$ times larger than that at off resonance. The transmission coefficient T_N can be written in the form

$$\begin{aligned} T_N(E) &= |Z_N(E)|^2 \\ &= \exp(-4\kappa l)\frac{\{1-[1-\exp(-2\kappa l)]^{N+1}\}^2+4[1-\exp(-2\kappa l)]^{N+1}\sin^2[(N+1)\phi/2]}{\exp(-4\kappa l)+4[1-\exp(-2\kappa l)]\sin^2(\phi/2)} . \end{aligned} \tag{16}$$

For the case where scattering is strong, i.e., $(N+1)\exp(-2\kappa l) \ll 1$, with the aid of the physics of diffraction gratings,[14] we obtain the transmission peak T_{Nr} as

$$T_{Nr}=\frac{1}{4}\left[\frac{\tau}{\tau_0}\right]^2 , \tag{17}$$

the ratio of the full width at half maximum for the strong scattering case (Γ_N) to that for the coherent case (Γ_∞) as

$$\frac{\Gamma_N}{\Gamma_\infty}=5.52\frac{\tau_0}{\tau} , \tag{18}$$

and the integrated transmission ratio I_N/I_∞ as

$$\frac{I_N}{I_\infty}=\frac{T_{Nr}\Gamma_N}{\Gamma_\infty}=1.38\frac{\tau_0}{\tau} , \tag{19}$$

where we introduce the intrinsic time constant τ_0 associated with Γ_∞ by

$$\tau_0=\frac{\hbar}{\Gamma_\infty} .$$

Detailed derivation of Eqs. (17), (18), and (19) is described elsewhere.[15] It is important to note that the peak current is decreased by τ/τ_0 for the strong scattering case.

Concerning this, we wish to describe the sequential tunneling proposed by Luryi.[4] His assertion is that negative differential resistance can arise due to electron tunneling into quasibound states in the well. As is easily seen from the above discussion, any quasibound state can be formed only due to multiple reflections in the well. Therefore, assuming the quasibound states indicates that multiple reflections (the Fabry-Perot effect) occur in the assumed system. In other words, Luryi's model of sequential tunneling which assumes the quasibound states in the well includes the Fabry-Perot effect implicitly. We can say that, until now, there has been some ambiguity as to what is called sequential tunneling. We here define sequential tunneling as the (t_0) process in Fig. 1(b), which includes no periodic paths in the well. Then we can see that negative differential resistance never arises from the sequential tunneling.

This conclusion can also be derived by using the uncertainty principle. Suppose that electrons with resonance energy E_r are incident to the double-barrier structure. For sequential tunneling dwell time Δt in the well is given by

$$\Delta t=\frac{L}{v} .$$

From the uncertainty principle ($\Delta E \Delta t \geq \hbar$), we have energy uncertainty ΔE as

$$\Delta E \geq \frac{2}{\alpha}E_r , \tag{20}$$

where we introduce a dimensionless number α of the order of unity by

$$E_r=\frac{\hbar^2}{2m}\left[\frac{\alpha}{L}\right]^2 ,$$

and use Eq. (14). Equation (20) indicates that for sequential tunneling the width of the energy level in the well is broadened to the energy level itself and that no discrete energy levels exist in the well.

The fact that the measured peak current is smaller than the calculated current can be interpreted as it is with the strong scattering case. Further, we can explain the fast response of the resonant tunneling diode, noting that the mean dwell time in the well is

$$\Delta t = 2N\frac{L}{v} . \tag{21}$$

The reflection coefficient can be calculated in a similar manner to the transmission coefficient, referring to Fig. 1(c),

$$R(E) = [1-\exp(-2\kappa l)]|1-\exp(i\phi)Z_\infty|^2 .$$

We can easily verify that, at resonance, $R=0$, which is consistent with the result for transmission. Thus we obtain the well-known result that, under resonance condition, the transmitted waves are all in phase and interfere constructively and that the reflected waves interfere destructively. However, looking at the reflection processes in detail, the paths from r_1 to r_∞ are all in phase and interfere constructively, and their contribution just cancels that of r_0.

We finally consider the phase shift accompanying reflection. In the discussion so far, we have assumed that the phase shift is $\frac{1}{2}\pi$ per one reflection. This value is equivalent to that obtained by the WKB approximation[16] which does not describe well the case with rectangular barriers. For this case, the exact phase shift χ can be obtained using the wave mechanics,[16,17]

$$\chi = 2\tan^{-1}\left[\left[\frac{V_0-E}{E}\right]^{1/2}\right] .$$

Then the resonance condition is modified as

$$\frac{1}{\hbar}\int_{x_1}^{x_2} p\, dx'' - \chi = n\pi .$$

This equation gives the same exact resonance energy as that obtained by solving the Schrödinger equation for this system.[17]

In summary, we have derived Feynman's path-integral formulation for resonant tunneling. The role of the semiclassical electron trajectories in resonant tunneling becomes clear. It is shown that multiple reflections in the well are necessary to produce negative differential resistance.

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