Effect of self-interference of an electron in motion: Analysis of nonlocality of an electron through a resonant tunneling diode

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On the basis of the viewpoint that a static wave function is formed as a result of self-interference of a moving electron, we investigate the temporal behavior of an electronic wave function through a resonant tunneling diode. In order to do it, we extend the WKB method by introducing a semiclassical orbital function so that we can follow the motion of an incident electron within a semiclassical picture. Within this theory, resonant tunneling is described as self-interference of amplitudes multiply reflected between potential barriers. We show that the components of multiply reflected amplitudes arrive with time delay, and thus total transmission amplitude is built up with time. At the resonant condition, the transmission probability is unity, implying that an electron behaves as if it senses beyond the barrier where the amplitude of a wave function is zero. This paradoxical nonlocality is reasonably understood in terms of the temporal buildup of transmission amplitudes due to multiple reflection.

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I. INTRODUCTION

The resonant tunneling diode (RTD) has been one of the staples of physics and device technologies using semiconductor nanostructures.

Figure 1 shows a schematic diagram of a RTD. The inset shows static transmission and reflection probabilities plotted as functions of electron energy, calculated by using the method described later in this paper. As is well known, tunneling probability is unity at the resonant condition; an incident electron travels through the double-barrier structure without decay when the electronic energy coincides with one of the energies of the quasibound states in the quantum well region. Of course, we cannot expect such a high transmission rate in real systems. However, the perfect transmission at resonance is a theoretical consequence in an ideal situation.

There are a large number of theoretical and experimental studies on RTD's in various conditions.[1] The properties of RTD's have been well revealed owing to these studies. For example, effects such as interface roughness scattering[2] and interaction between electrons[3] in the tunneling current have been studied. Not only conventional RTD's, but the resonant effect in Zener tunneling has also been observed.[4–6]

However, we may encounter an embarrassing situation. Let us think that an incident electron is expressed as a localized wave packet. If we have a naive interpretation of the tunneling probability, the transmission rate of 100% at resonance (accordingly a zero reflection rate) means that an electron arriving at the edge of the barrier keeps on moving as if there is no barrier. However, such behavior of an electron is quite mysterious; why does the electron know that there is a quasibound state beyond the barrier? There is no amplitude of the incident electron in the quantum well region before penetration through the barrier occurs. This nonlocality contradicts naive intuition.

In order to explain such nonlocal behavior of a tunneling electron, a theoretical framework beyond conventional treatments is necessary. As far as we know, no clear answer to the question has been given, though there are many theoretical studies on the temporal behavior of tunneling electrons.[7–15] We will show in this paper that the nonlocality is reasonably

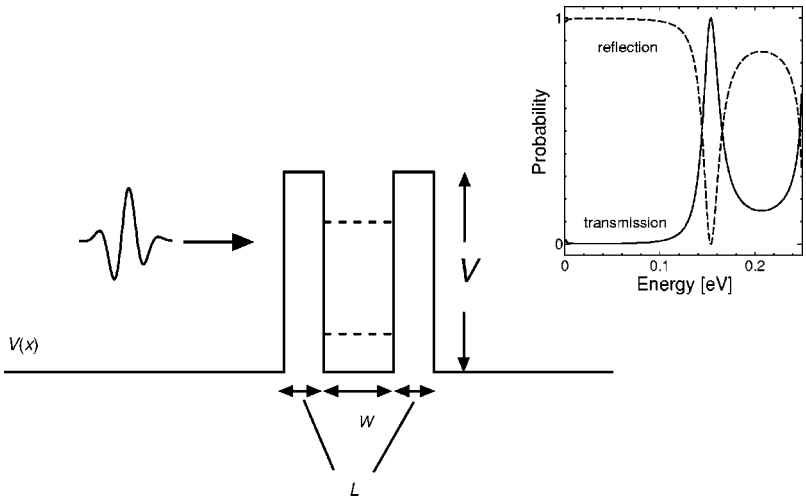

FIG. 1. Schematic diagram of a resonant tunneling diode. Quasibound states in the well region are shown by the dashed horizontal lines. Inset: Transmission and reflection probabilities calculated within the method described in Sec. II.

understood by considering the temporal behavior and self-interference of an electron.

There are various techniques to investigate the motion of an electron.[10,11,16] By using one of the techniques, we can describe the time evolution of an electronic state through potential barriers, solving the time-dependent Schrödinger equation numerically. With numerical analysis, however, we may miss physical insight as a price for accuracy. On the other hand, the WKB method provides us a clear physical picture of the resonant tunneling phenomenon,[17] although numerical errors are inevitable.

In this study, we apply the WKB method in order to grasp the physics of the temporal behavior of tunneling electrons. We develop a theory on the basis of the perspective that a static wave function is formed due to self-interference of a moving electron. In Sec. II, we extend the WKB approximation based on the path-integral theory, so that we can treat the dynamics of a tunneling electron. Numerical results calculated based on the extended WKB approximation are shown and discussed in Sec. III.

We note that temporal analysis of tunneling electrons is also interesting from the viewpoint of device application. It is necessary to evaluate the tunneling probability on a short time scale, so as to investigate characteristics of RTD's under a high-frequency alternating voltage.[18–21]

II. ELECTRON DYNAMICS BASED ON THE WKB METHOD

A. The WKB approximation within the path-integral theory

First in this section, we review the WKB approximation which is often used for analysis of tunneling phenomena.[17,22] Within the path-integral theory, the time evolution of an electron is given by

$$\psi(x,t) = \int_{-\infty}^{\infty} K(x,t;x_0,t_0)\psi(x_0,t_0)dx_0, \tag{1}$$

where $\psi(x_0,t_0)$ is the wave function at an initial time t_0, and $K(x,t;x_0,t_0)$ is a function called a Feynman kernel.[23–25] In the WKB approximation, the Feynman kernel is given by

$$K(x,t;x_0,t_0) = \sum_a \sqrt{\frac{i}{2\pi\hbar}\frac{\partial^2 S_{cl}^{\alpha}}{\partial x\,\partial x_0}}\, e^{iS_{cl}^{\alpha}/\hbar + i\eta^{\alpha}}, \tag{2}$$

where S_{cl}^{α} is the action evaluated along a semiclassical path (specified with an index α) connecting the initial point (x_0,t_0) and the final point (x,t) of electron's motion. Some of the possible paths for resonant tunneling are depicted in Fig. 2, where r and t stand for reflection and transmission, respectively. In Eq. (2), η^{α} denotes the change of phase factor accompanied by singular points in the paths. For a double-barrier structure, a jump of potential acts as a singularity. A wave function thus undergoes a phase change when it passes through (or is reflected by) a potential step. Values of η^{α} will be discussed in the next section and the appendixes. If the incident state $\psi(x_0,t_0)$ has a well-defined position, we may follow the motion of this state by using Eq. (1).

We consider an incident electron with energy E. Here we introduce a function defined by

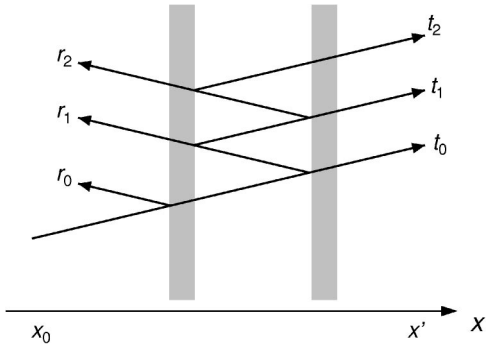

FIG. 2. Some of possible paths of an electron through a double-barrier structure. The potential barriers are indicated by the gray regions, and r and t stand for reflection and transmission, respectively.

$$\chi_E(x,t) = \int_{t_0}^{t} e^{iE\tau/\hbar}\psi(x,\tau)d\tau. \tag{3}$$

Mathematically, Eq. (3) can be regarded as a Fourier transformation, changing the variable from time to energy. We may, however, interpret it as the afterimage of a moving electron; a coherent superposition of time-evolving wave functions.[26,27] In this sense, the function $\chi_E(x,t)$ has a meaning as a time-integrated probability amplitude, i.e., the probability of finding an electron during the period $t_0 \sim t$.[28]

The exponential function in Eq. (3) is necessary to have a reasonable result. It cancels the time-dependent phase factor of $\psi(x,\tau)$, which is $e^{-iE\tau/\hbar}$. Such cancellation is necessary from the viewpoint of gauge invariance of $\chi_E(x,t)$. When we consider a coherent superposition of wave functions belonging to different times, an additional constant potential will change the relative phase difference between the wave functions. As a result, the superposed function becomes quite different by the choice of origin of the energy axis. Such a situation is irrational and undesirable. Thus, the time-dependent phase factor of a moving state must be excluded from the superposition as shown in Eq. (3).

By inserting Eqs. (1) and (2) into Eq. (3), we have

$$\begin{aligned}\chi_E(x,t) &= \int_{-\infty}^{\infty}\left[\int_{t_0}^{t} e^{iE\tau/\hbar}K(x,\tau;x_0,t_0)d\tau\right]\psi(x_0,t_0)dx_0 \\ &= c\sum_{\alpha}\int_{t_0}^{t} d\tau\sqrt{\frac{i}{2\pi\hbar}\frac{\partial^2 S_{cl}^{\alpha}}{\partial x\,\partial x_0}}\, e^{i(E\tau+S_{cl}^{\alpha})/\hbar + i\eta^{\alpha}}\end{aligned} \tag{4}$$

with $c=(4\pi/a)^{1/4}$. To obtain the second expression, we set the initial state localized as

$$\psi(x_0,t_0) = \left(\frac{a}{\pi}\right)^{1/4} e^{-ax^2/2} \simeq \left(\frac{4\pi}{a}\right)^{1/4}\delta(x_0) \tag{5}$$

with sufficiently large a. We note that the function in the square bracket $[\cdots]$ in the first line of Eq. (4) corresponds to energy representation of the Feynman kernel, which is defined by

$$K_E(x,x_0) = \lim_{t-t_0\to\infty} \frac{1}{i\hbar}\int_{t_0}^{t} e^{iE\tau/\hbar}K(x,\tau;x_0,t_0)d\tau. \quad (6)$$

When the initial state $\psi(x_0,t_0)$ is localized at x_0 as shown in Eq. (5), χ_E and K_E are essentially equivalent except for a constant factor. Instead of K_E, however, we will use the function χ_E in the following formulation so as to stress that the Fourier transformation by time is an expression of self-interference of a moving electron.

We can evaluate the time integration of Eq. (4) by a method called the stationary phase approximation. Since $\hbar$ is a small quantity, the exponential function in Eq. (4) oscillates quickly with time. Thus, we can expect that the time integration vanishes unless the argument of the exponential function is extremum. This means that we can evaluate the time integration from the values at the extrema, which are called stationary points.

By utilizing this idea, we approximate the exponential function in Eq. (4) by expanding S_{cl}^{α} around the stationary point up to the second order as

$$e^{i(E\tau+S_{cl}^{\alpha})/\hbar} \simeq \exp\left\{\frac{i}{\hbar}\left[W^{\alpha}(x,x_0;E) + \frac{1}{2}\frac{\partial^2 S_{cl}^{\alpha}}{\partial\tau^2}(\tau-\overline{\tau})^2\right]\right\}. \quad (7)$$

In this equation, the stationary point $\overline{\tau}$ is obtained from

$$E + \left.\frac{\partial S_{cl}^{\alpha}}{\partial\tau}\right|_{\tau=\overline{\tau}} = 0, \quad (8)$$

and the function $W^{\alpha}(x,x_0;E)$ is

$$W^{\alpha}(x,x_0;E) = E\overline{\tau} + S_{cl}^{\alpha}|_{\overline{\tau}} = \int_{x_0}^{x}\sqrt{2m^*[E-V(x')]}dx' \quad (9)$$

for a potential $V(x)$. The integration in Eq. (9) is carried out along a path α.

As an example of Eq. (8), we show the case for a free electron. The action due to free motion is

$$S_{cl}^{\alpha} = \frac{m^*}{2}\frac{(x-x_0)^2}{\tau}. \quad (10)$$

Equation (8) then results in the relation

$$x(\overline{\tau}) = x_0 + \sqrt{\frac{2E}{m^*}}\overline{\tau}, \quad (11)$$

where $\sqrt{2E/m^*}$ is velocity. Such a relation enables us to define the path of an electron. Regarding the stationary point $\overline{\tau}$ as an independent time variable, Eq. (11) gives the electron's position as a function of time,

By inserting Eq. (7) into Eq. (4) and extending the bounds of integration to $-\infty<\tau<\infty$, we have[17,22]

$$\begin{aligned}\chi_E(x) &= c\sum_{\alpha}\sqrt{\frac{i}{2\pi\hbar}\frac{\partial^2 S_{cl}^{\alpha}}{\partial x\,\partial x_0}}e^{iW^{\alpha}/\hbar+i\eta^{\alpha}} \\ &\quad\times\int_{-\infty}^{\infty}\exp\left(\frac{i}{\hbar}\frac{1}{2}\frac{\partial^2 S_{cl}}{\partial\tau^2}(\tau-\overline{\tau})^2\right)d\tau \\ &= c\sqrt{-\frac{\partial^2 S_{cl}^{\alpha}/\partial x\,\partial x_0}{\partial^2 S_{cl}^{\alpha}/\partial\tau^2}}e^{iW^{\alpha}/\hbar+i\eta^{\alpha}} \\ &= c\left|\frac{\partial^2 W^{\alpha}}{\partial E\,\partial x}\frac{\partial^2 W^{\alpha}}{\partial E\,\partial x_0}\right|^{1/2}e^{iW^{\alpha}/\hbar+i\eta^{\alpha}} = \sum_{\alpha}\chi_E^{\alpha}(x), \quad (12)\end{aligned}$$

with

$$\chi_E^{\alpha}(x) = c\left|\frac{\partial^2 W^{\alpha}}{\partial E\,\partial x}\frac{\partial^2 W^{\alpha}}{\partial E\,\partial x_0}\right|^{1/2}e^{iW^{\alpha}/\hbar+i\eta^{\alpha}}. \quad (13)$$

The function $\chi_E^{\alpha}(x)$ is the electronic amplitude through a path α. Hence, Eq. (12) means that the amplitude of an electron at the point x is expressed as a superposition of amplitudes from semiclassical paths. We note that a single electron travels through *all the paths*. Summation of amplitudes from all the paths governs the electron's behavior.

We also note that these results can be applied even for $E\leqslant V(x)$ where an electron is in a potential barrier.[17,29] In this case, electron velocity is given by

$$v = \sqrt{\frac{2}{m^*}[V(x)-E]}, \quad (14)$$

within the semiclassical picture.

B. Extension of the WKB method for electron dynamics

We can investigate the static properties of a tunneling electron using Eqs. (12) and (13), because $\chi_E(x)$ is essentially a static wave function.

We extend here the theory so as to describe the time evolution of an electron. Remember that Eqs. (12) and (13) were obtained by evaluating the time integration around a stationary point. In other words, $\chi_E(x)$ is a superposition of wave functions of a moving electron. We also note that the stationary point gives the semiclassical path of electronic motion as shown in Eq. (11). These facts lead us to the idea that it will be useful to introduce a wave function whose superposition along a semiclassical path yields $\chi_E^{\alpha}(x)$. Within the spirit of the WKB method, which is often called a semiclassical approximation, such a wave function should have a definite position, moving along a semiclassical path.

By considering these conditions, we define a function $\phi_E^{\alpha}(x^{\alpha}(\tau))$ with an equation

$$c\int_{t_0}^{t} e^{iE\tau/\hbar}\phi_E^{\alpha}(x^{\alpha}(\tau))d\tau = \chi_E^{\alpha}(x,t), \quad (15)$$

where $x^{\alpha}(\tau)$ is a semiclassical path.

When $\partial^2 S_{cl}/\partial\tau^2$ in Eq. (7) is large, we have an approximate relation

$$\exp\left(\frac{i}{\hbar}\frac{1}{2}\frac{\partial^2 S_{cl}}{\partial\tau^2}(\tau-\overline{\tau})^2\right) \simeq \sqrt{\frac{2\pi i\hbar}{\partial^2 S_{cl}/\partial\tau^2}}\delta(\tau-\overline{\tau}). \quad (16)$$

By inserting this equation into Eq. (7), Eq. (4) becomes

$$\chi_E(x,t) = c\sum_\alpha \int_{t_0}^{t} d\tau \sqrt{-\frac{\partial^2 S_{cl}^\alpha/\partial x\,\partial x_0}{\partial^2 S_{cl}^\alpha/\partial\tau^2}}\, e^{iW^\alpha/\hbar + i\eta^\alpha}\delta(\tau-\overline{\tau}). \quad (17)$$

Therefore we have

$$\phi^\alpha(x^\alpha(\tau)) = \left|\frac{\partial^2 W^\alpha}{\partial E\,\partial x}\frac{\partial^2 W^\alpha}{\partial E\,\partial x_0}\right|^{1/2} e^{i(W^\alpha - E\tau)/\hbar + i\eta^\alpha}\delta(\tau-\overline{\tau}), \quad (18)$$

from comparison between Eq. (17) and Eq. (15).

The function $\phi_E^\alpha(x^\alpha(\tau))$ is a particlelike state moving along a semiclassical path. This function, thus, is regarded as a compromise between quantum and classical views.

We may estimate the spatial extension length of $\phi^\alpha(x^\alpha(\tau))$ with

$$\Delta x \simeq \sqrt{\frac{2E}{m^*}} \times \sqrt{\frac{\hbar\overline{\tau}}{E}}. \quad (19)$$

In this equation, the first factor is the velocity and the second factor is the temporal extent given by

$$\frac{1}{\Delta_t^2} \simeq \frac{1}{2\hbar}\left.\frac{\partial^2 S_{cl}}{\partial\tau^2}\right|_{\overline{\tau}} = \frac{E}{\hbar\overline{\tau}}, \quad (20)$$

where Eq. (10) was used. By using typical values $\overline{\tau}=10$ fs and $m^*=9.1\times10^{-31}$ kg, we have $\Delta x\simeq 14$ Å.

In the following calculations, however, we treat $\phi^\alpha(x^\alpha(\tau))$ as a particlelike function, neglecting the spatial extent. This approximation allows us to define unambiguous paths near the potential steps.

III. TIME ANALYSIS OF AN ELECTRON THROUGH A RESONANT TUNNELING DIODE

In Fig. 3, we show an example of behavior of a single electron described by the theory shown in the previous section. We carried out calculations for a double-barrier structure with structural parameters $L=20$ Å, $W=60$ Å, and $V=250$ meV. Considering GaAs as a host material, the mass of an electron is $0.068\,m_0$ with the electron rest mass m_0.

The upper panel shows the function $\phi_E^\alpha(x^\alpha(t))$ moving along the path t_0, traveling through the potential barriers without any reflection. The energy of the electron is 150 meV. We note that the functions at each time are plotted by Gaussian curves instead of a δ function for the purpose of visualization. The electron initially located at $x=-200$ Å moves toward the right with changing phase. Passing through the potential barriers (denoted by the gray zones) with decay of amplitude, it reaches the position $x=220$ Å at $t=46$ fs.

As for the phase change due to singularities η^α, we adopt

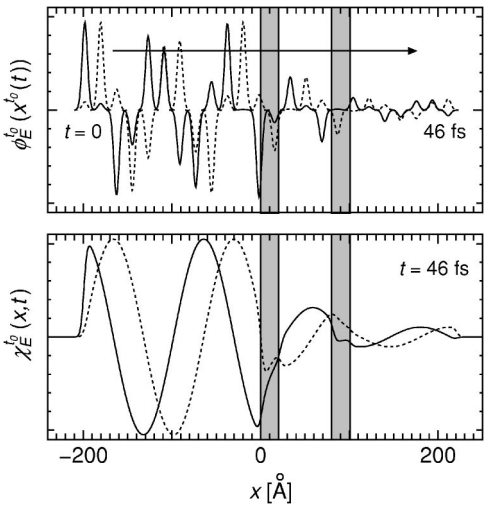

FIG. 3. Upper panel: The Gaussian curves denote the function $\phi_E^\alpha(x^\alpha(t))$ moving along the path t_0 which directly tunnels through the double-barrier structure. Electron energy and effective mass are 150 meV and $0.068m_0$, respectively. The electron at $x=-200$ Å at $t=0$ reaches the position 220 Å at 46 fs. Lower panel: The function $\chi_E^\alpha(x,t)$ at $t=46$ fs is plotted. Note that this function has a value only in the region where the electron passed through. In these figures, the solid and dashed curves are for the real and imaginary parts, respectively, and the potential barriers are indicated by the gray regions.

$$\eta^\alpha = n\frac{\pi}{4} + n'\pi, \quad (21)$$

where n (n') is the number of times the electron passes through (is reflected by) a potential step. As shown in Appendixes A and B, this treatment gives rise to resonant energies $E_n=(\hbar^2/2m^*)(n\pi/W)^2$ with $n=1,2,\ldots$ as expected for an ideal quantum well. In addition, unitarity for scattered amplitudes is satisfied with these values of the phase change. It is known that phase change due to a singular point is $\pi/2$ within the WKB method. However, it has been proven that this value is unsuitable for an abrupt potential step.[30] See Appendixes A and B for the details about the effect of phase change on resonant energies.

The lower panel of Fig. 3 shows the function $\chi_E^{t_0}(x,t)$ defined by Eq. (15), corresponding to the motion shown in the upper panel. We note that the plotted function has a value only in the region where the electron passed through, because electron motion in a finite region is considered. This function thus has a meaning similar to a scar. As we have noted in the previous section, this function is essentially a static wave function.

In Fig. 4, the functions $e^{iEt/\hbar}\phi_E^\alpha(x^\alpha(t))$ for the transmission paths t_0, t_1, and t_2 are plotted with offset. The function $\chi_E^\alpha(x,t)$ corresponding to each path is given as an envelope of the moving wave functions. Since the total transmission amplitude is the summation of the $\chi_E^\alpha(x,t)$'s for all paths, a large value of the transmission amplitude is realized when the $e^{iEt/\hbar}\phi_E^\alpha(x^\alpha(t))$'s are in phase. On the other hand, when the phases of the components from the paths are different, the

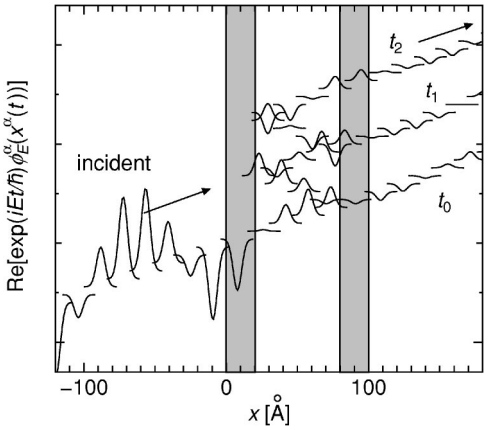

FIG. 4. Motion of a localized wave function along some paths for a double-barrier structure. t_0 indicates a path that directly tunnels through the barriers. t_1 and t_2 are paths multiply reflected between the barriers.

amplitudes cancel with one another. As a result, in this case, the total transmission amplitude becomes small.

A similar illustration for typical reflection paths is shown in Fig. 5, where the $e^{iEt/\hbar}\phi_E^\alpha(x^\alpha(t))$'s for reflection paths r_0 and r_1 are plotted with offset. Based on the same argument as shown above, the total reflection amplitude becomes large (small) due to constructive (destructive) interference among amplitudes from the paths.

An important consequence of the present theory is that the amplitudes from multiply reflected paths arrive with time delay. This is because an electron spends some time in the quantum well region while it is multiply reflected. Owing to such time delay of amplitudes, the total transmission and reflection amplitudes are built up gradually with time.

In order to see the temporal behavior of a tunneling electron, we calculated time-dependent transmission coefficients defined by

$$T_E(x,t) = \frac{\chi_E^{(t)}(x,t)}{\chi_E^{(in)}(x_0)}. \tag{22}$$

In this equation, $\chi_E^{(t)}(x,t)$ denotes the amplitude of transmission given by

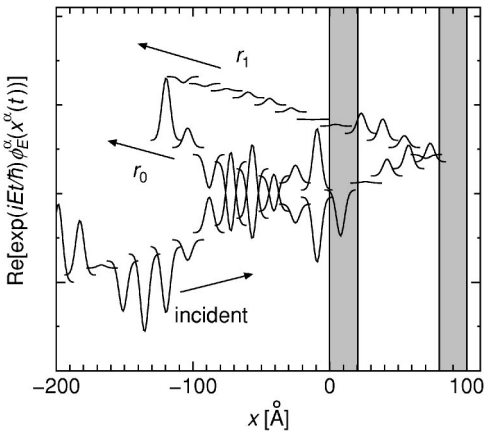

FIG. 5. Motion of a wave packet along some paths. $r_0(r_1)$ indicates a path reflected by the first (second) barrier.

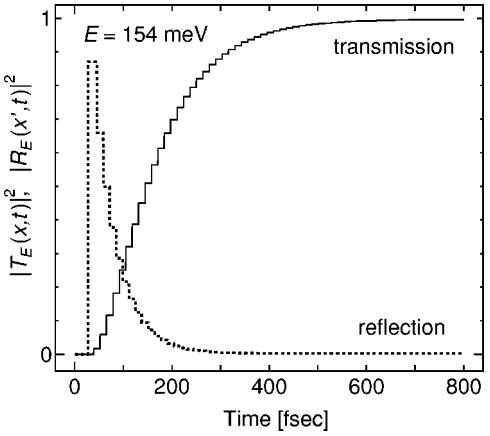

FIG. 6. Time dependence of probability amplitude for transmission and reflection. Electron energy is 154 meV, which is the resonant energy for the present double-barrier structure.

$$\chi_E^{(t)}(x,t) = \sum_\alpha{}' \int_{\bar{t}}^{t} e^{iE\tau/\hbar}\phi_E^\alpha(x^\alpha(\tau))d\tau, \tag{23}$$

where $\bar{t}$ is the time when the electron reaches the first barrier. The summation over α is taken for the transmission paths. The denominator

$$\chi_E^{(in)}(x) = \int_{t_0}^{\bar{t}} e^{iE\tau/\hbar}\phi_E^\alpha(x^\alpha(\tau))d\tau \tag{24}$$

is the amplitude of the incident state.

Similarly, we define a time-dependent reflection coefficient as

$$R_E(x',t) = \frac{\chi_E^{(r)}(x',t)}{\chi_E^{(in)}(x_0)}, \tag{25}$$

with reflection amplitude $\chi_E^{(r)}(x',t)$ defined in a similar way to Eq. (23).

In Fig. 6, we show the time-dependent transmission and reflection probabilities by the solid and dotted curves, respectively. In the calculations, we have evaluated the transmission amplitude at the position $x=150$ Å, and the reflection amplitude at $x'=-50$ Å. The electron energy 154 meV corresponds to the resonant energy for the present double-barrier structure. In this case, the transmission amplitude becomes larger bit by bit as other components from the multiply reflected path arrive at the position x. Finally it becomes unity, corresponding to transmission without decay. Simultaneously with the behavior of the transmission amplitude, the reflection amplitude becomes gradually smaller as a result of the superposition of multiply reflected components. Although the reflection amplitude has a large value at the early stage because of the direct reflection component from r_0, it finally becomes zero.

Such behavior of the reflection amplitude gives a clear reasonable answer to the question of nonlocality we have mentioned in the Introduction. Even though the reflection probability is zero, it does not mean that an electron behaves as if there is no barrier. An electron does not sense beyond the barrier where its amplitude is zero. Even in the condition

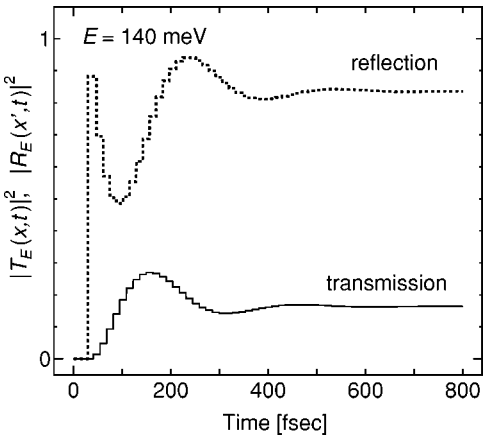

FIG. 7. Time dependence of probability amplitude for transmission and reflection calculated for electron with energy 140 meV.

of perfect resonance where the reflection probability is zero, the electron is reflected by the potential barrier. Multiply reflected components cancel out the total reflection amplitude with time until it becomes zero.

In Fig. 7, we show transmission and reflection amplitudes calculated for an off-resonant energy $E=140$ meV. In this case, the superposition of multiply reflected amplitudes gives rise to oscillation of the transmission and reflection probabilities until they reach steady values. The transmission and reflection probabilities shown in the inset of Fig. 1 are such steady values plotted as functions of energy. We note that unitarity is not satisfied in transitive time, though it is satisfied in the long time limit.

It is known that the charge of resonant tunneling electrons stays in the quantum well region for a considerably long time.[12,13] The charge in the well decreases slowly with time. This fact corresponds to the present result that the transmission and reflection amplitudes approach steady values with time.

Recently, the time-dependent current through a double-barrier structure has been calculated by using Green's functions.[15] The calculated current shows temporal oscillation, which is similar to the behavior of the transmission amplitude shown in Fig. 7.

In many quantum mechanical calculations, electronic properties are investigated by solving a static Schrödinger equation. Resonant tunneling is also often analyzed with steady-state wave functions. However, the present results show that electron dynamics is necessary to understand the essence of a phenomenon such as resonant tunneling.

As shown in this paper, the resonant tunneling is a quantum mechanical phenomenon which arises from interference of amplitudes from various paths. The present theory well describes this aspect. However, as for the electron motion along each path, the present method is based on the semiclassical picture where an electron has definite position and momentum. We have followed the motion of an electron within the WKB method and stationary phase approximation. With these methods, we have regarded an electron as a localized particlelike state. With a strict treatment of quantum mechanics, however, a localized wave function becomes extended with time. We have to note that this effect is neglected in the present theory. Therefore the behavior of the probability amplitudes shown in Figs. 6 and 7 has to be somewhat rectified if we consider the spatial extension of moving states exactly.

IV. CONCLUSION

We investigated the temporal behavior of an electron through a double-barrier structure by extending the WKB method. Based on the viewpoint that a static wave function is formed due to self-interference, a steady-state wave function is expressed as a coherent superposition of wave functions of a moving electron. The transmission and reflection amplitudes are given by summations of amplitudes from semiclassical paths corresponding to multiple reflection in the quantum well region. Since multiply reflected components arrive one by one with time delay, the total amplitudes for transmission and reflection of an electron are built up with time.

This result provides us a reasonable interpretation for the nonlocal character of tunneling electron noted in the Introduction. Perfect transmission (and zero reflection) at resonance does not mean that the electron is not scattered by the barrier. The refection amplitude approaches zero with time as a result of interference of multiply reflected components. Zero reflection does not mean that an electron senses beyond the barrier where its amplitude is zero.

We have to note that the calculated results in this theory have some numerical deviation from exact values. The WKB method which we employed is valid only for high-energy electrons. It gives rise to numerical errors. As a result, the method shown in this paper may be unsuitable for analysis of real devices.

However, we can expect that gross features of the calculated time dependence of the amplitudes are qualitatively reasonable, and that the present theory will be useful to describe physics of electron dynamics in nanostructures.

APPENDIX A: RESONANT ENERGY AND PHASE CHANGE AT A POTENTIAL BARRIER

In this appendix, we show that the phase change of a wave function at a potential barrier is closely related to the resonant condition.

First, we consider transmission and reflection at a single square barrier of width L and height V. We write the tunneling coefficient as

$$t = e^{-\kappa L + i\varphi}, \tag{A1}$$

with $\kappa=\sqrt{2m^*(V-E)}/\hbar$. The coefficient for reflection is then given by

$$r = e^{i\varphi'}\sqrt{1-|t|^2}, \tag{A2}$$

so that $|t|^2+|r|^2=1$ is satisfied. In Eqs. (A1) and (A2), φ and φ' are phase changes associated with tunneling and reflection, respectively.

Next, we consider double barriers separated by W. By considering multiple reflection in the quantum well region, the total transmission coefficient is given by a geometric series as

$$t_{\text{total}}(E) = t^2 e^{i\theta} + t^2 r^2 e^{3i\theta} + t^2 r^4 e^{5i\theta} + \cdots = \frac{t^2 e^{i\theta}}{1-(1-|t|^2)e^{2i\varphi'+2i\theta}}, \quad \text{(A3)}$$

where $\theta = \sqrt{2mE}W/\hbar$ is the electron's phase change across the quantum well. The condition for resonant tunneling is given by

$$\theta + \varphi' = n\pi, \quad \text{(A4)}$$

because this equation results in $t_{\text{total}}(E)$ as

$$t_{\text{total}}(E) = \frac{t^2 e^{i\theta}}{|t|^2} = e^{2i\varphi+i\theta}, \quad \text{(A5)}$$

giving $|t_{\text{total}}(E)|^2 = 1$.

Within the WKB theory, $\pi/2$ of phase change due to reflection is often imposed. If we apply $\varphi' = \pi/2$ for Eq. (A4), the resonant energy is obtained as

$$E_n = \frac{\hbar^2}{2m^*}\left[\frac{(n-1/2)\pi}{W}\right]^2. \quad \text{(A6)}$$

By using $\varphi' = \pi$ instead of $\pi/2$, we have

$$E_n = \frac{\hbar^2}{2m^*}\left(\frac{n\pi}{W}\right)^2, \quad \text{(A7)}$$

which is a reasonable result.

By considering this result, in this paper we have adopted the phase change at reflection $\varphi' = \pi$ because Eq. (A6) has an additional factor $1/2$ for energy levels in the quantum well region. On the other hand, Eq. (A7) gives a plausible value for the energies of states in the quantum well. However, we have to note that numerical solution of the Schrödinger equation is necessary to obtain exact resonant energies associated with the exact phase change due to reflection.

APPENDIX B: CONDITION FOR UNITARITY

Similarly to Eq. (A3), the total reflection amplitude is given by

$$r_{\text{total}}(E) = r + rt^2 e^{2i\theta} + t^2 r^3 e^{4i\theta} + t^2 r^5 e^{6i\theta} + \cdots = r + \frac{rt^2 e^{2i\theta}}{1-(1-|t|^2)e^{2i\varphi'+2i\theta}}. \quad \text{(B1)}$$

At the resonance condition Eq. (A4), $r_{\text{total}}(E)$ is

$$r_{\text{total}}(E_n) = r + \frac{rt^2 e^{2i\theta}}{|t|^2} = r(1+e^{2i\varphi+2i\theta}). \quad \text{(B2)}$$

From the requirement of unitarity, $|t_{\text{total}}|^2 + |r_{\text{total}}|^2 = 1$ must be satisfied. Therefore $r_{\text{total}}(E_n) = 0$ must be satisfied for the resonant energies E_n. Thus, from Eqs. (A4) and (B2), the phase changes for transmission and reflection should satisfy the relation

$$\varphi - \varphi' = \pm\pi/2. \quad \text{(B3)}$$

This relation is satisfied by imposing a phase change $\pi/4$ when an electron passes through a potential step.

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