

Tunneling time based on the quantum diffusion process approach in multi-channel and optical potential cases

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Abstract. We analyze the effects of inelastic scattering on the tunneling time theoretically, using generalized Nelson's quantum mechanics. This generalization enables us to describe quantum system with channel couplings and optical potential in a real time stochastic approach, which seems to give us a new insight into quantum mechanics beyond Copenhagen interpretation.

Keywords. Tunneling time; stochastic approach; quantum mechanics.

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1. Introduction

An issue of the tunneling time has been discussed in many theoretical studies [1] and is not settled yet. This difficulty arises mainly from the fact that time is not an observable represented by a self-adjoint operator but just a parameter in quantum mechanics.

In our previous paper [2], we proposed a new method to evaluate the tunneling time, using Nelson's approach of quantum mechanics [3]. It has several advantages to study the tunneling time. First of all, this approach enables us to describe individual experimental runs of a quantum system in terminology of "analogue" of classical mechanics. This is true even in the tunnel region where classical path is forbidden. From sample paths generated by the stochastic process we obtain information on the time parameter, in particular, the tunneling time. It is important for us to note that in scattering phenomena the transmission and reflection ensembles are defined unambiguously. In numerical simulations we need to accumulate a sufficient number of sample paths. In thick or/and high potential case the transmission probability is low and consequently we have a difficulty that a number of sample paths belonging to the transmission ensemble is also low. However, in Nelson's approach, this difficulty is avoided when the backward Langevin equation is employed.

Taking account of these advantages, we have developed a formulation of time-dependent description of tunneling phenomena based on the Nelson's approach in [2]. Numerical simulations for a one-dimensional square well potential barrier model were demonstrated. An

important result then is that there are the three characteristic times, i.e., *the passing time* and *the hesitating time*, and their sum, *the interacting time*. The probability distribution of these three times were calculated numerically.

In this paper we consider cases in which transition processes into other channels or absorptive processes takes place during scattering processes, and look into these effects on the tunneling time. The purpose of this paper is to generalize the Nelson's stochastic quantization so that it can deal with multi-channel coupling and/or optical potential problems. As will be shown below, one can construct such generalized formulations of the Nelson's approach with additional *stochastic jumping processes*.

We show a brief review of the Nelson's quantum mechanics. The quantum process for a coordinate variable is represented by the Ito-type stochastic differential equations for forward time evolution,

$$dx(t) = b(x(t), t)dt + dw(t), \tag{1}$$

and for backward time evolution,

$$dx(t) = b_*(x(t), t)dt + dw_*(t). \tag{2}$$

The $dw(t)$ is the Gaussian white noise with the statistical properties of $\langle dw(t) \rangle = 0$ and $\langle dw(t)dw(t) \rangle = \frac{\hbar}{m}dt$, and the same properties for $dw_*(t)$. Here $\langle \dots \rangle$ means a sample average. It is easy to show that for these two Langevin equations hold the following Fokker-Planck equations for the distribution function $P(x, t)$ of the random variable $x(t)$,

$$\frac{\partial P(x, t)}{\partial t} = \left[-\frac{\partial}{\partial x}b(x, t) + \frac{\hbar}{2m} \frac{\partial^2}{\partial x^2} \right] P(x, t) \quad (\text{forward in } t), \tag{3}$$

$$-\frac{\partial P(x, t)}{\partial t} = \left[\frac{\partial}{\partial x}b_*(x, t) + \frac{\hbar}{2m} \frac{\partial^2}{\partial x^2} \right] P(x, t) \quad (\text{backward in } t). \tag{4}$$

Thus a pair of equations (1) and (2) is mathematically equivalent to a pair of equations (3) and (4). We get an osmotic velocity, u from the sum of eqs (3) and (4) as

$$u = \frac{b - b_*}{2} = \frac{\hbar}{2m} \frac{1}{P} \frac{\partial P}{\partial x}. \tag{5}$$

The subtraction (4) from (3) gives a continuity equation and a current velocity, v as

$$\frac{\partial P}{\partial t} = -\frac{\partial}{\partial x}(vP), \quad v = \frac{b + b_*}{2}. \tag{6}$$

The elimination of $P(x, t)$ from (5) and (6) leads to an equation called the kinematical equation,

$$\frac{\partial u}{\partial t} = -\frac{\hbar}{2m} \frac{\partial^2 v}{\partial x^2} - \frac{\partial}{\partial x}(uv). \tag{7}$$

The dynamical condition is expressed through the "mean balanced acceleration"

$$a(x(t), t) \equiv \frac{DD_* + D_*D}{2}x(t) = -\frac{\hbar}{2m} \frac{\partial^2 u}{\partial x^2} + \frac{1}{2} \frac{\partial}{\partial x}(v^2 - u^2) + \frac{\partial v}{\partial t}. \tag{8}$$

Here $D(D_*)$ is "mean forward(backward) time derivative". The dynamical condition is nothing but the classical Newton equation to this "mean balanced acceleration" $a(x(t), t)$, $ma(x, t) = -\frac{\partial V}{\partial x}$, from which we derive the "Newton-Nelson equation",

$$\frac{\partial v}{\partial t} = \frac{\hbar}{2m} \frac{\partial^2 u}{\partial x^2} - v \frac{\partial v}{\partial x} + u \frac{\partial u}{\partial x} - \frac{1}{m} \frac{\partial V}{\partial x}. \tag{9}$$

The kinematical condition (7) and the dynamical condition (9) form a set of simultaneous equations for two unknown functions $u(x, t)$ and $v(x, t)$, or equivalently $b(x, t)$ and $b_*(x, t)$. Then we can determine the ensemble of sample paths or the distribution function $P(x, t) = |\psi(x, t)|^2$. One can easily show the equivalence between this approach and the ordinary approach of the Schrödinger equation.

2. Stochastic formulation for quantum system with channel coupling

Let us consider the 2-channel Schrödinger equations ($\{i, j\} = \{1, 2\}$), for simplicity,

$$i\hbar \frac{\partial}{\partial t} \psi_i(x, t) = \left(-\frac{\hbar^2}{2m_i} \frac{\partial^2}{\partial x^2} + V_{ii}(x, t) \right) \psi_i(x, t) + V_{ij}(x, t) \psi_j(x, t), \quad V_{ij} = V_{ji}^*. \quad (10)$$

Hereafter the dummy index does not imply taking a sum. Consider the corresponding Fokker–Planck equations in the stochastic formulation. First we require a natural extension of the distribution function to the present case, $P_i(x, t) = |\psi_i(x, t)|^2$. The Schrödinger equations (10) and their complex conjugates suggest the following equations for $P_i(x, t)$,

$$\frac{\partial P_i(x, t)}{\partial t} = \left[-\frac{\partial}{\partial x} b_i(x, t) + \frac{\hbar}{2m_i} \frac{\partial^2}{\partial x^2} - W_{(i \rightarrow j)}(x, t) \right] P_i(x, t) \quad (\text{forward}), \quad (11)$$

$$-\frac{\partial P_i(x, t)}{\partial t} = \left[\frac{\partial}{\partial x} b_{*i}(x, t) + \frac{\hbar}{2m_i} \frac{\partial^2}{\partial x^2} + W_{(i \rightarrow j)}(x, t) \right] P_i(x, t) \quad (\text{backward}). \quad (12)$$

$P_i(x, t)$ increases or decreases, due to the potential V_{ij} causing transitions between i and j , at the rate of the absolute value of

$$W_{(i \rightarrow j)} P_i = -W_{(j \rightarrow i)} P_j = \frac{2}{\hbar} \text{Im} \psi_j^* V_{ji} \psi_i \quad (13)$$

Although the sum of (11) and (12) leads to (5) with the index i ,

$$u_i = \frac{b_i - b_{*i}}{2} = \frac{\hbar}{2m_i} \frac{1}{P_i} \frac{\partial P_i}{\partial x}, \quad (14)$$

their difference provides us with

$$\frac{\partial P_i}{\partial t} = -\frac{\partial}{\partial x} (v_i P_i) - W_{(i \rightarrow j)} P_i, \quad v_i = \frac{b_i + b_{*i}}{2}. \quad (15)$$

Eliminating $P_i(x, t)$ from (14) and (15), one derives the following kinematical equation

$$\frac{\partial u_i}{\partial t} = -\frac{\hbar}{2m_i} \frac{\partial^2 v_i}{\partial x^2} - \frac{\partial}{\partial x} (u_i v_i) - \frac{\hbar}{2m_i} \frac{\partial}{\partial x} W_{(i \rightarrow j)}. \quad (16)$$

Here arises a natural question what are stochastic differential equations corresponding to the Fokker–Planck equations. Apparently we need two random variables $x_i(t)$ ($i = 1, 2$),

which are assumed to be subject to the stochastic differential equations, similar to (1) and (2),

$$dx_i(t) = b_i(x_i(t), t)dt + dw_i(t) \quad (\text{forward in time}), \quad (17)$$

$$dx_i(t) = b_{*i}(x_i(t), t)dt + dw_{*i}(t) \quad (\text{backward in time}), \quad (18)$$

with the properties for $dw_i(t)$, $\langle dw_i(t) \rangle = 0$ and $\langle dw_i(t)dw_j(t) \rangle = \frac{\hbar}{m_i} \delta_{ij} dt$, and the same properties for $dw_{*i}(t)$. Furthermore, an additional mechanism is necessary to take account of the quantum jump between i and j represented by the terms involving $W_{(i \rightarrow j)}$. For this purpose we supplement (17) and (18) with a stochastic jumping process between i and j .

The rule is described by the following random jumping process (figure 1): At each time a dice is cast, independently of the stochastic equation (17) and (18), and each sample path either keeps or changes its index at a certain rate. For forward time direction, we have the rule in case of $W_{(i \rightarrow j)} > 0$ ($i \neq j$),

$$\begin{aligned} x_i(t) &\longrightarrow \begin{cases} x_j(t + dt) & \text{with the probability of } W_{(i \rightarrow j)}(x_i(t), t)dt, \\ x_i(t + dt) & \text{with the probability of } 1 - W_{(i \rightarrow j)}(x_i(t), t)dt, \end{cases} \\ x_j(t) &\longrightarrow x_j(t + dt) \quad \text{with the probability of } 1, \end{aligned} \quad (19)$$

and the rule in case of $W_{(i \rightarrow j)} < 0$

$$\begin{aligned} x_j(t) &\longrightarrow \begin{cases} x_i(t + dt) & \text{with the probability of } -W_{(i \rightarrow j)}(x_j(t), t)dt, \\ x_j(t + dt) & \text{with the probability of } 1 + W_{(i \rightarrow j)}(x_j(t), t)dt, \end{cases} \\ x_i(t) &\longrightarrow x_i(t + dt) \quad \text{with the probability of } 1. \end{aligned} \quad (20)$$

Likewise, we have the rules for backward time direction.

Due to changes in the index for each sample path, there are several types of averages which are distinguished from each other carefully. It is convenient to introduce notations for conditional averages. The simple average $\langle \cdot \cdot \rangle$ should be taken over both of $dw_1(s)$ and $dw_2(s)$ ($s < t$). To represent a physical average of the i -state at t , we introduce a notation of

$$\langle \langle f(x(t)) \rangle \rangle_{\{x_i(t)\}} \equiv \langle f(x_i(t)) \rangle = \int dx f(x) P_i(x, t), \quad (21)$$

where the average on the left-handed side implies a conditional average only over sample paths, labeled by i at t . The notation $\langle \langle f(x(t)) \rangle \rangle_{\{x_1(t)\} \cup \{x_2(t)\}}$ owns its trivial interpretations, $\langle f(x(t)) \rangle$. Furthermore, conditional averages with different times such as $\langle \langle f(x(t)) \rangle \rangle_{\{x_i(t+dt)\} \cap \{x_j(t)\}}$ can be introduced. Let us now evaluate the time derivative of the physical average $\langle \langle f(x(t)) \rangle \rangle_{\{x_i(t)\}}$. For forward time direction, using appropriate conditional averages, we write down as

$$\begin{aligned} &\langle \langle f(x(t + dt)) \rangle \rangle_{\{x_i(t+dt)\}} - \langle \langle f(x(t)) \rangle \rangle_{\{x_i(t)\}} \\ &= \langle \langle f(x(t + dt)) - f(x(t)) \rangle \rangle_{\{x_i(t+dt)\} \cap \{x_i(t)\}} \\ &\quad + \langle \langle f(x(t + dt)) \rangle \rangle_{\{x_i(t+dt)\} \cap \{x_j(t)\}} \\ &\quad - \langle \langle f(x(t)) \rangle \rangle_{\{x_j(t+dt)\} \cap \{x_i(t)\}} \end{aligned} \quad (22)$$

The three terms in r.h.s. are manipulated according to (19) and (20). The final form is

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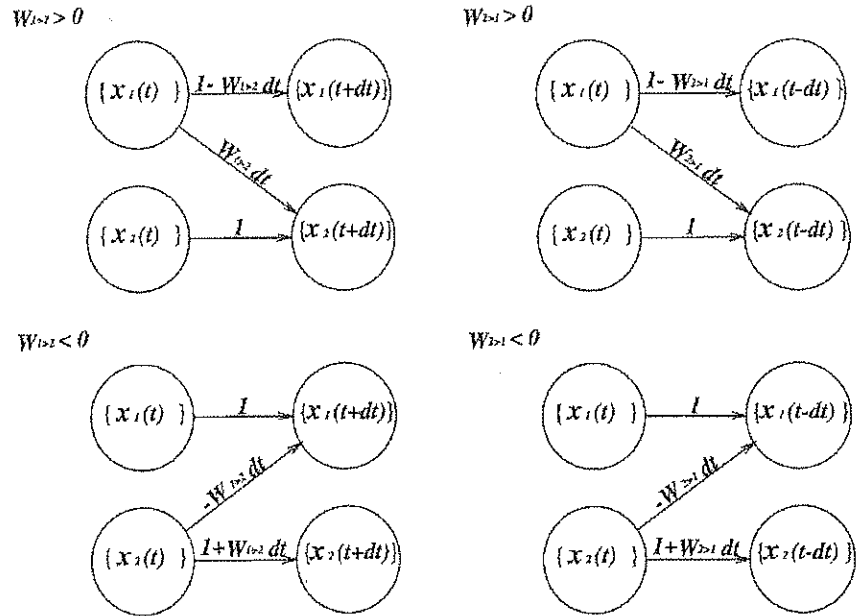


Figure 1. Schematic illustration of the “dynamical” rule for stochastic jumping process between two channels.

$$\begin{aligned}
 & \langle \langle f(x(t+dt)) \rangle \rangle_{\{x_i(t+dt)\}} - \langle \langle f(x(t)) \rangle \rangle_{\{x_i(t)\}} \\
 &= dt \int dx f(x) \left(-\frac{\partial}{\partial x} b_i(x, t) \right. \\
 & \quad \left. + \frac{\hbar}{2m_i} \frac{\partial^2}{\partial x^2} - W_{(i \rightarrow j)}(x, t) \right) P_i(x, t) + o(dt^2). \quad (23)
 \end{aligned}$$

This gives us the correct time evolution of (11) and shows the equivalence between (11) and (17) supplemented with the stochastic jumping process (19) and (20).

For the equivalence between the Nelson’s approach and the Schrödinger approach, the dynamical condition is desired to have the form of

$$\frac{\partial v_i}{\partial t} = \frac{\hbar}{2m_i} \frac{\partial^2 u_i}{\partial x^2} - v_i \frac{\partial v_i}{\partial x} + u_i \frac{\partial u_i}{\partial x} - \frac{1}{m_i} \frac{\partial \tilde{V}_{ii}}{\partial x}. \quad (24)$$

Here we introduce a “quantum potential” \tilde{V}_{ii} which is to include the effect of channel coupling as well as the usual potential V_{ii} . The simplest way to achieve this equation is to define the “mean balanced acceleration” a_i through the “mean (forward and backward) time derivative” as usual but for the stochastic process without any jumping process. Using the “mean balanced acceleration” $a_i(x_i(t), t)$ defined in this way, we define the “Newton” equations,

$$m_i a_i(x_i(t), t) = -\frac{\partial \tilde{V}_{ii}}{\partial x_i}, \quad (25)$$

from which we get (24).

The combination of the equations (16)+i(24) derives

$$\frac{\partial}{\partial x} \left[i \frac{\hbar}{m} \frac{1}{\psi'_i} \frac{\partial \psi'_i}{\partial t} + \frac{1}{2} \left(\frac{\hbar}{m_i} \right)^2 \frac{1}{\psi'_i} \frac{\partial^2 \psi'_i}{\partial x^2} - \frac{1}{m_i} \left\{ \tilde{V}_{ii} - \frac{i\hbar}{2} W_{(i \rightarrow j)} \right\} \right] = 0 \quad (26)$$

where the relation,

$$u_i + iv_i = \frac{\hbar}{m_i} \frac{1}{\psi'_i} \frac{\partial \psi'_i}{\partial x}, \quad (27)$$

is used. If we shift the function ψ'_i to

$$\psi_i(x, t) = \psi'_i(x, t) \exp\left(-\frac{im_i}{\hbar} \int^t \eta(s) ds\right), \quad (28)$$

choose the “quantum potential” as

$$\tilde{V}_{ii} = V_{ii} + \text{Re} \frac{\psi_i^* V_{ij} \psi_j}{|\psi_i|^2}, \quad (29)$$

and use the relation (13)

$$W_{(i \rightarrow j)} = -\frac{2}{\hbar} \text{Im} \frac{\psi_i^* V_{ij} \psi_j}{|\psi_i|^2}, \quad (30)$$

we can reproduce the Schrödinger equations (10). By the use of the (27) and (28), the relations,

$$b_i(x, t) = \frac{\hbar}{m_i} (\text{Im} + \text{Re}) \frac{\partial}{\partial x} \ln \psi_i(x, t) \quad (31)$$

$$b_{*i}(x, t) = \frac{\hbar}{m_i} (\text{Im} - \text{Re}) \frac{\partial}{\partial x} \ln \psi_i(x, t) \quad (32)$$

$$P_i(x, t) = |\psi_i(x, t)|^2 \quad (33)$$

are obtained.

3. Stochastic formulation for quantum system of optical potential

The Schrödinger equation with an imaginary part of potential, denoted by iU (an absorptive process corresponds to $U < 0$), is written down as

$$i\hbar \frac{\partial \psi(x, t)}{\partial t} = \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x, t) + iU(x, t) \right) \psi(x, t). \quad (34)$$

The analogy between the channel coupling model and the present model becomes apparent when we attempt to have the corresponding Fokker-Planck equation,

$$\frac{\partial P(x, t)}{\partial t} = \left[-\frac{\partial}{\partial x} b + \frac{\hbar}{2m} \frac{\partial^2}{\partial x^2} + \frac{2U}{\hbar} \right] P(x, t) \quad (\text{forward in } t), \quad (35)$$

$$-\frac{\partial P(x, t)}{\partial t} = \left[\frac{\partial}{\partial x} b_* + \frac{\hbar}{2m} \frac{\partial^2}{\partial x^2} - \frac{2U}{\hbar} \right] P(x, t) \quad (\text{backward in } t). \quad (36)$$

While the sum of (35) and (36) is given by (5), their difference leads to

$$\frac{\partial P}{\partial t} = -\frac{\partial}{\partial x}(vP) + \frac{2U}{\hbar}P. \quad (37)$$

From (5) and (37), follows the kinematical equation

$$\frac{\partial u}{\partial t} = -\frac{\hbar}{2m} \frac{\partial^2 v}{\partial x^2} - \frac{\partial}{\partial x}(uv) + \frac{1}{m} \frac{\partial}{\partial x}U. \quad (38)$$

Equations (35) and (36) are compared with (11) and (12), then both are quite similar to each other with the correspondence between $2U/\hbar$ and $-W_{(i \rightarrow j)}$. This is more obvious through the introduction of an “unphysical” sector. One may put inelastic effects in a such way that the absorption(production) process is a transition from a “physical” sector to an “unphysical” sector (vice versa). We consider the two random variables $x_p(t)$ and $x_u(t)$ for “physical” and “unphysical” sectors, respectively. Introducing a notation of a random variable $x(t)$ for both of $x_p(t)$ and $x_u(t)$, we require the same form of stochastic differential equations for this $x(t)$ as (1) and (2) *all the time*. Each sample path is described by $x(t)$ as a whole, but has to be classified into either $x_p(t)$ or $x_u(t)$ at each t . We can give “dynamical” rule for stochastic jumping processes between p and u as is illustrated in figure 2. Then one can easily prove the equivalence between the Fokker–Planck equation (35) and the stochastic differential equation (1) supplemented with the jumping rules.

As for the dynamical condition, we do not modify the original Nelson’s formulation and have the “Newton–Nelson equation” in (9) in the present case. The combination of the equations (38)+i(9) leads to

$$\frac{\partial}{\partial x} \left[i \frac{\hbar}{m} \frac{1}{\psi'} \frac{\partial \psi'}{\partial t} + \frac{1}{2} \left(\frac{\hbar}{m} \right)^2 \frac{1}{\psi'} \frac{\partial^2 \psi'}{\partial x^2} - \frac{1}{m} (V + iU) \right] = 0 \quad (39)$$

where the relation (27) without index is used.

4. Numerical analysis

First, we discuss one-dimensional system with a static square well optical potential,

$$V(x) = \begin{cases} 0 & \text{in I} & (x < 0), \\ V_0 - iU_0 & \text{in II} & (0 < x < d), \\ 0 & \text{in III} & (d < x). \end{cases} \quad (40)$$

We set the solution of the Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} \psi(x, t) = \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right] \psi(x, t) \quad (41)$$

as

$$\psi(x, t) = \int_{-\infty}^{\infty} A(k) \varphi_k(x) e^{-i\frac{E}{\hbar}t} dk \quad (42)$$

with a coefficient function $A(k)$ and $E = \frac{\hbar^2 k^2}{2m}$. We take a Gaussian form with its center at $k = k_0$, $A(k) = A_{k_0}(k) = C \exp \left\{ -\frac{(k_0 - k)^2}{4\sigma^2} \right\}$, with a normalization constant C . We put here $\sigma = \frac{k_0}{100}$ and $V_0 = 5E_0 = \left(\frac{\hbar k_0}{2m} \right)^2$.

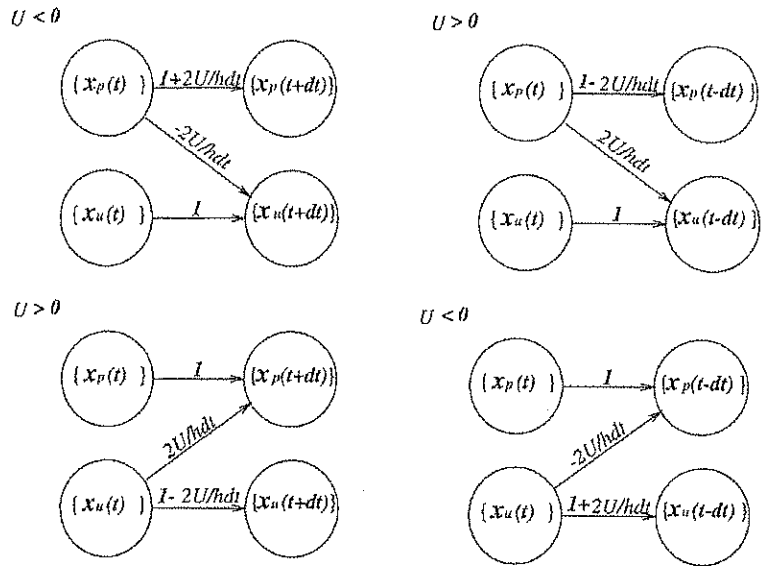


Figure 2. Schematic illustration of “dynamical” rule for stochastic jumping process between physical and unphysical sector.

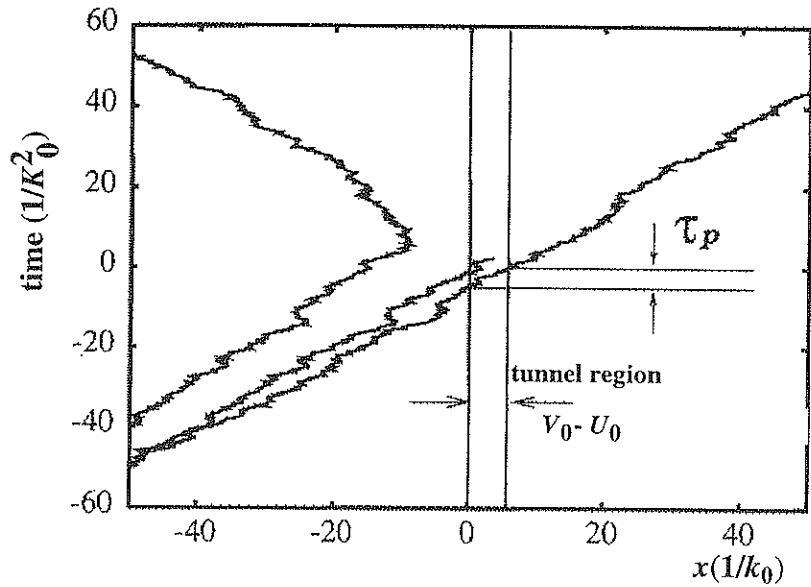


Figure 3. The three typical sample paths in the optical potential case.

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Figure 3 shows the three typical sample paths. There is a sample path $x(t)$ which changes its property from “physical” to “unphysical” in the tunnel region. Figures 4 and 5 shows the parameter $\frac{U_0}{E_0}$ v.s. the average of passing time τ_p . See the details of this

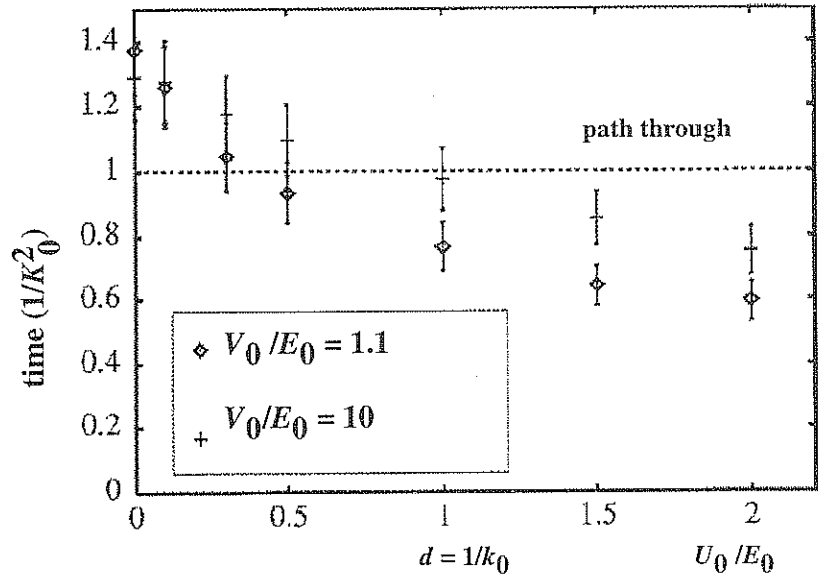


Figure 4. The mean value of τ_p versus $\frac{U_0}{E_0}$ (thin potential cases).

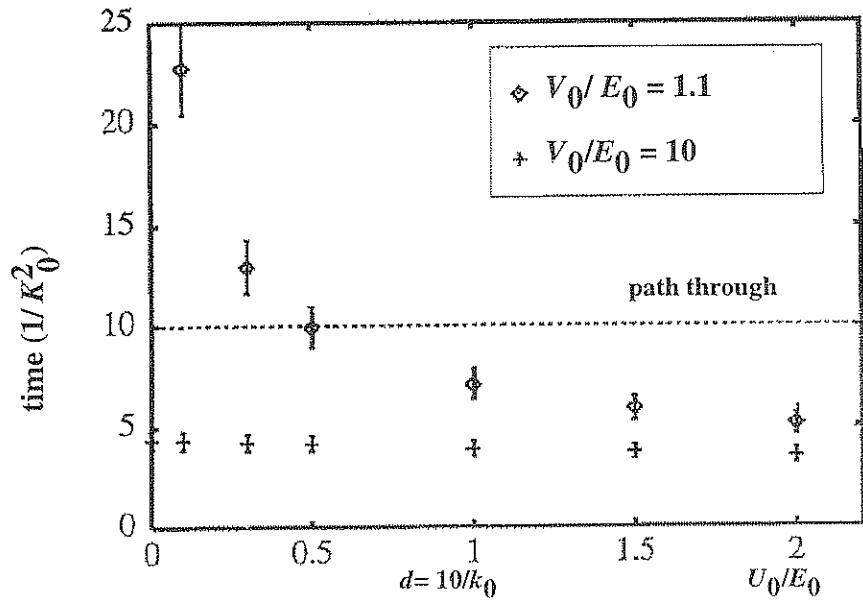


Figure 5. The mean value of τ_p versus $\frac{U_0}{E_0}$ (thick potential cases).

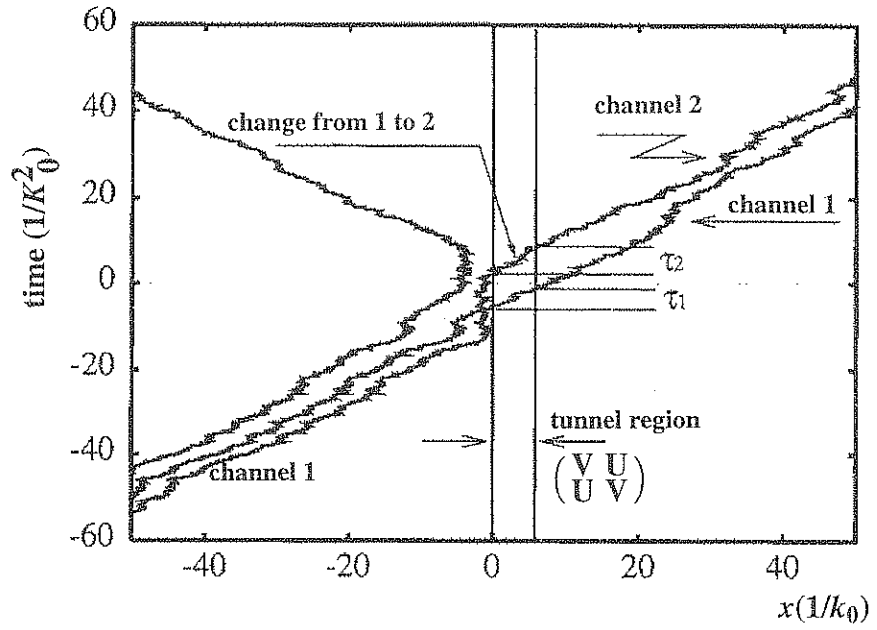


Figure 6. The three typical sample paths with the the channel coupling.

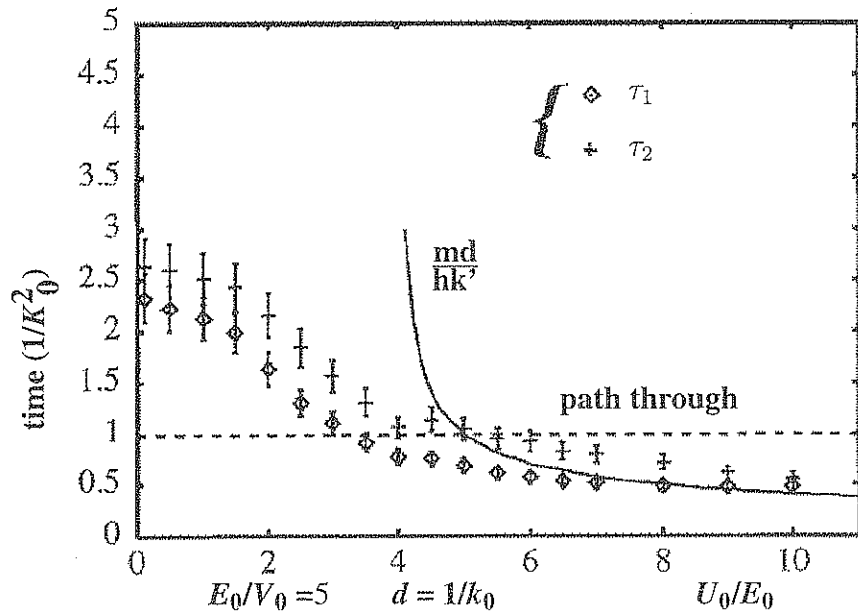


Figure 7. The mean values of τ_1 and τ_2 versus $\frac{U_0}{E_0}$ (thin potential cases).

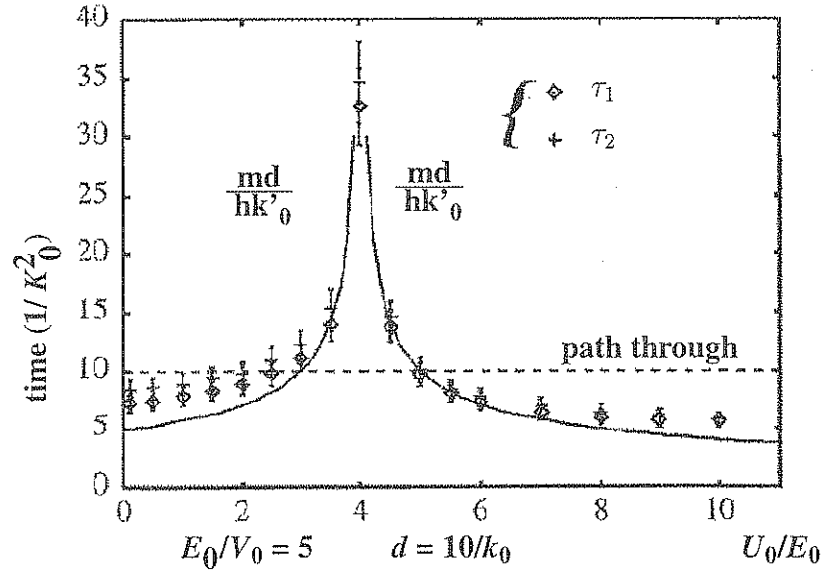


Figure 8. The mean values of τ_1 and τ_2 versus $\frac{U_0}{E_0}$ (thick potential cases).

“backward time evolution method” in our previous work [2]. Generally, τ_p decrease as the $\frac{U_0}{E_0}$ become larger.

Secondly, we discuss a one-dimensional system with a static square well potential and 2-channel coupling, or the case of the Schrödinger equation for this problem written down as

$$i \frac{\partial}{\partial t} \begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix} = \begin{bmatrix} -\frac{1}{2m} \frac{\partial^2}{\partial x^2} + V & U \\ U & -\frac{1}{2m} \frac{\partial^2}{\partial x^2} + V \end{bmatrix} \begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix}. \quad (43)$$

Real potentials V and U have similar forms as (40) with heights of V_0 and U_0 . Figure 6 shows some typical sample paths calculated by (17), (19) and (20). There is a path which changes its index from 1 to 2 in the passage through the tunneling region. $\tau_i = 1, 2$ Figures 7 and 8 are the averages of the passing times over the sample paths which belong to $\{x_i(t)\}$ at $t \rightarrow \infty$.

5. Summary and comments

In this paper, we have analyzed the effects of inelastic scattering on the tunneling time theoretically, using generalized Nelson’s quantum mechanics. This generalization enables us to describe quantum system with channel couplings and optical potential in a real time stochastic approach. In this formalism, the space-time development of dynamical vari-

able, e.g. coordinate of particle, is described by a definite path determined stochastically. Each sample path has a definite form of trajectory in space-time diagram, while a physical quantity averaged over the ensemble of these sample paths recovers the effect of quantum coherence. This is true even in the Young's double slits interference experiment. Nelson's quantum mechanics gives each definite trajectory and the ensemble of it, but it does not predict which path is selected when one wants to measure the position of a particle. In this sense, this "real time stochastic process approach" seems to give us a new insight into quantum mechanics beyond Copenhagen interpretation.

Recent experimental data of tunneling time using the neutron spin echo shift through the magnetic films [4] seem to agree with the simulation based on our approach [5] and this study will be reported in near future.

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