Potential renormalization by tunneling induced intrinsic transition

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The screening effects by bound target electrons in low energy nuclear reactions in laboratory experiments can be well represented in terms of a constant shift of the tunneling potential barrier as postulated in all previous analyses if the electronic cloud were static or structureless and lied outside the tunneling region. In this paper, using a semiclassical mean field analysis of a simple two-level coupled-channels problem, we suggest that there could occur a strong quantum transition of electrons from excited to the ground states in the tunneling region, leading to a spatially dependent screening potential. We thus show the necessity of the dynamical treatment of the tunneling region in order to properly assess the screening effects by bound target electrons in low energy nuclear reactions in laboratories.

I. INTRODUCTION

The rate of nuclear reactions at extremely low energies in laboratory experiments shows a marked enhancement over the extrapolation from high energy data$^1$. This phenomenon has been attributed to the screening effect by the bound electrons in the target nucleus, and has been discussed in many papers for almost a decade. Yet, a clear understanding is missing. A standard approach is to analyze the data by assuming that the electrons lead to a constant potential shift in the tunneling region, which is called the screening energy. A surprise is that the phenomenological value of the screening energy thus obtained exceeds the so called adiabatic limit, which is conventionally given by the difference between the binding energies in the target and the united atoms and is thought to give the maximum screening energy, for all systems so far studied. One should, however, be aware of the fact that a spatially constant potential renormalization can be justified only for a static electronic cloud, namely, when the electronic state makes no transition in the tunneling region.

The screening problem can be understood as an example of the so called macroscopic quantum tunneling, where intrinsic degrees of freedom affect the tunneling probability of a macroscopic variable, by considering the electrons and the relative motion between the projectile and target nuclei as the intrinsic and macroscopic degrees of freedom, respectively. In this paper, we show that a strong intrinsic transition can happen to facilitate the tunneling probability leading to a novel, spatially dependent potential renormalization. In order to demonstrate this, we use a simple two-level coupled-channels problem and analyze the associated tunneling process based on a semi-classical mean field theory, which naturally describes the effects of intrinsic degrees of freedom on the quantum tunneling of a macroscopic variable in terms of a potential renormalization.

The paper is organized as follows. In sect.2, we briefly describe the essence of the semi-classical mean field theory for quantum tunneling and apply it to a two-level coupled-channels problem. In sect.3, we examine the accuracy of the semi-classical mean field theory through the comparison of the barrier transmission probability given by the semiclassical mean field theory with that obtained by a direct numerical solution of the coupled-channels equations. In sect.4, we discuss the properties of the transition of the intrinsic state and the associated potential renormalization. We summarize the paper in sect.5.

II. SEMICLASSICAL MEAN FIELD THEORY FOR QUANTUM TUNNELING

A. Basic coupled-equations

Our interest is to study the time evolution of a system, which consists of a macroscopic variable $X$ which undergoes a quantum tunneling and intrinsic degrees of freedom $\xi$. In the screening problem, the former and the latter correspond to the coordinate of the relative motion between the projectile and target nuclei and electronic degrees of freedom, respectively, if one ignores the intrinsic structure of nuclei.
We assume that the time dependent Schrödinger equation for the total system is given by,

\[ i\hbar \frac{\partial \Psi(X, \xi, t)}{\partial t} = [H_N(X) + H_0(\xi) + V(X, \xi)] \Psi(X, \xi, t) \] (1)

where we used the notation \( H_N(X) \) for \(-\frac{\hbar^2}{2\mu} \frac{\partial^2}{\partial X^2} + U(X)\), \( U(X) \) being the bare interaction between the projectile and target nuclei. The \( H_0(\xi) \) and \( V(X, \xi) \) represent the unperturbed Hamiltonian of the electrons and the interaction between the electrons and nuclei.

We now approximate \( \Psi(X, \xi, t) \) by a product of the wave functions for the macroscopic and intrinsic motions

\[ \Psi(X, \xi, t) = \phi(\xi, t)\eta(X, t) \] (2)

and determine the wave function in each space based on the following variational principle,

\[ \frac{\delta \mathcal{L}}{\delta \phi^*(\xi, t)} = 0 \] (3)

\[ \frac{\delta \mathcal{L}}{\delta \eta^*(X, t)} = 0 \] (4)

where the Lagrangian is defined by

\[ \mathcal{L} = \int_{t_0}^{T} dt \langle \phi \eta | (i\hbar \frac{d}{dt} - H) | \phi \eta \rangle \] (5)

We call this approach a mean field theory or a Hartree approximation (see [2, 3] for details).

One can try to numerically solve the resultant time dependent coupled-equations for \( \phi(\xi, t) \) and \( \eta(X, t) \). However, as is well known [4], that approach is adequate to describe only the classically allowed region. It suffers from the so-called spurious correlation effect to handle the tunneling region. As a practical method to circumvent this problem, we treat the macroscopic motion classically and resort to the imaginary time approach to describe the tunneling process. Identifying the classical variables with the expectation values of the corresponding operators at each time, we have the following coupled equations for the classically allowed region

\[ i\hbar \frac{\partial \phi(\xi, t)}{\partial t} = [H_0(\xi) + V(X(t), \xi)] \phi(\xi, t), \] (6)

\[ \mu \frac{\partial^2}{\partial \tau^2} X(t) = - \frac{\partial}{\partial X} [U(X) + \frac{\langle \phi(t) | [H_0 + V(X(t), \xi)] | \phi(t) \rangle}{\langle \phi(t) | \phi(t) \rangle}] \] (7)

They lead to the following energy conservation law

\[ \frac{1}{2} \mu \left( \frac{\partial}{\partial t} X(t) \right)^2 + U(X(t)) + \frac{\langle \phi(t) | [H_0 + V(X(t), \xi)] | \phi(t) \rangle}{\langle \phi(t) | \phi(t) \rangle} = E. \] (8)

where the total energy \( E \) is given by the sum of the initial kinetic energy \( E_K \) and the initial intrinsic energy \( \epsilon_0 \).

As already mentioned, we describe the tunneling process using the imaginary time \( t = -i\tau \). We must, however, find also the proper way to describe the effects of intrinsic motion during the tunneling process. For example, it is not obvious whether the potential renormalization is given by the same expression as that in eq.(6) or one should replace \( \langle \phi(t) | \phi(t) \rangle \) by the adjoint state. We discuss in a separate paper [3] the effective potential equivalent to the dynamical norm factor which takes non adiabatic effect into account and show that the proper generalization of eqs.(6) through (8) to the tunneling region are given by

\[ \hbar \frac{\partial \phi(\xi, \tau)}{\partial \tau} = - [H_0(\xi) + V(X(\tau), \xi)] \phi(\xi, \tau), \] (9)

\[ \mu \frac{\partial^2}{\partial \tau^2} X(\tau) = \frac{\partial}{\partial X} [U(X) + \frac{\langle \phi(\tau) | [H_0(\xi) + V(X, \xi)] | \phi(\tau) \rangle}{\langle \phi(\tau) | \phi(\tau) \rangle}], \] (10)

\[ - \frac{1}{2} \mu \frac{\partial}{\partial \tau} X(\tau)^2 + U(X(\tau)) + \frac{\langle \phi(\tau) | [H_0 + V(X(\tau), \xi)] | \phi(\tau) \rangle}{\langle \phi(\tau) | \phi(\tau) \rangle} = E, \] (11)
We see in eqs. (7) and (10) the explicit expression of the potential renormalization in the classical and tunneling regions, respectively.

**B. Application to a two-level coupled-channels problem**

We now apply the semi-classical mean field theory to a coupled-channels problem, which has proved to be very powerful to discuss, e.g., the effects of nuclear intrinsic degrees of freedom on the cross section of heavy-ion fusion reactions at energies below the Coulomb barrier [6]. Here we consider a simple model, where the intrinsic motion has two levels

$$H_0 |\phi_m\rangle = \epsilon_m |\phi_m\rangle \quad (m = 1, 2),$$

and the coupling Hamiltonian is separable

$$V(X, \xi) = f(X) \cdot \hat{M}(\xi).$$

Expanding the total wave function on the basis of intrinsic states

$$\Psi = \sum_m \eta_m(X) |\phi_m(\xi)\rangle,$$

one obtains the following coupled equations to describe the macroscopic motion

$$\left[ -\frac{\hbar^2}{2\mu} \frac{d^2}{dX^2} + U(X) - E \right] \begin{pmatrix} \eta_1(X) \\ \eta_2(X) \end{pmatrix} + \begin{pmatrix} \epsilon_1 & 0 \\ 0 & \epsilon_2 \end{pmatrix} \begin{pmatrix} \eta_1(X) \\ \eta_2(X) \end{pmatrix} + f(X) \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \begin{pmatrix} \eta_1(X) \\ \eta_2(X) \end{pmatrix} = 0.$$

In the direct method, these coupled-equations are numerically solved with the following boundary conditions,

$$\eta_n(X) \to \frac{1}{\sqrt{k_n}} e^{-ik_n X} \quad (X \ll 0)$$

$$\to \frac{1}{\sqrt{k_n}} [I_n e^{-ik_n X} + r_n e^{ik_n X}] \quad (X \gg 0),$$

where $k_n = \sqrt{2\mu (E - \epsilon_n)}$. The amplitude of the incident wave $I_n$ is taken to be $\delta_{nn}$ if the intrinsic motion is initially in the state $|\phi_n\rangle$. Once the transmission amplitudes $t_n$ are determined, the barrier transmission probability is given by,

$$P = \sum_n |t_n|^2.$$

In order to compare the results with those of the semi-classical mean field theory, the same problem can be cast into the form of the corresponding time dependent approach, where the wave function for the internal motion is expressed as

$$\phi(\xi, t) = a_1(t) \phi_1(\xi) + a_2(t) \phi_2(\xi) = a_1(t) \begin{pmatrix} 1 \\ 0 \end{pmatrix} + a_2(t) \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

Following eqs. (3) and (4), the expansion coefficients $a_1$ and $a_2$ obey

$$i\hbar \frac{d a_1(t)}{dt} = \epsilon_1 a_1(t) + f(X(t)) \{ M_{11} a_1(t) + M_{12} a_2(t) \}$$

$$i\hbar \frac{d a_2(t)}{dt} = \epsilon_2 a_2(t) + f(X(t)) \{ M_{21} a_1(t) + M_{22} a_2(t) \},$$

$(X \ll 0)$
in the classically allowed region, and

\[ -\hbar \frac{da_1(\tau)}{d\tau} = \epsilon_1 a_1(\tau) + f(X(\tau))\{M_{11}a_1(\tau) + M_{12}a_2(\tau)\} \tag{22} \]

\[ -\hbar \frac{da_2(\tau)}{d\tau} = \epsilon_2 a_2(\tau) + f(X(\tau))\{M_{21}a_1(\tau) + M_{22}a_2(\tau)\}, \tag{23} \]

in the tunneling region. Using thus obtained \(a_1\) and \(a_2\) the renormalization of the potential barrier for the macroscopic motion by internal degrees of freedom is given by

\[ \Delta V(X(t)) = \frac{\epsilon_1|a_1(t)|^2 + \epsilon_2|a_2(t)|^2 + \sum_{m,m'} M_{mm'} a_{m'}^*(t)a_{m'}(t) \cdot f(X)}{|a_1(t)|^2 + |a_2(t)|^2} - \epsilon_0 \tag{24} \]

in the classically allowed region. The same expression holds for the tunneling region by replacing \(a_i(t)\) with \(a_i(\tau)\), \(i\) being 1 and 2. Eqs. (20) and (21) or eqs. (22) and (23) should be solved together with eqs. (24) and (24), respectively, with the potential renormalization given by eq. (24) in the classically allowed region and the corresponding one in the tunneling region to determine the classical trajectory \(X(t)\) and \(X(\tau)\).

One then calculates the barrier transmission probability for each initial kinetic energy \(E_K\) by the WKB formula as

\[ P(E) = \exp\left(-\frac{4}{\hbar} \int_{\tau_a}^{\tau_b} d\tau [U(X(\tau)) + \Delta V(X(\tau)) - E_K]\right) \tag{25} \]

where \(\tau_a\) and \(\tau_b\) correspond to the inner and outer classical turning points, respectively, and the time integral is performed over the tunneling region.

### III. ACCURACY OF THE SEMICLASSICAL MEAN FIELD THEORY

Before we discuss the characteristics of the intrinsic transition and the associated potential renormalization, we examine in this section the reliability of the semi-classical mean field theory for quantum tunneling. We consider the case where the coupling matrix is given by

\[ M = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{26} \]

and assume that the bare potential and the coupling form factor have the Eckart form [3]

\[ U(X) = \frac{U_0}{\cosh^2(X/a)}, \quad f(X) = \frac{f_0}{\cosh((X-X_f)/a_f)}, \tag{27} \]

where the height of the potential barrier is fixed to be \(U_0 = 10\ MeV\), and the position of the coupling form factor \(X_f\) is taken to be either 50 \(fm\) in front of the central region of the potential barrier or 0 \(fm\). The large value of \(X_f\) is taken, because we can then clearly separate the transition of the intrinsic state by the coupling form factor and by the tunneling effect. The latter transition and the associated potential renormalization, i.e. the potential renormalization induced by the tunneling assisted intrinsic transition are the major issues which we wish to advocate in this paper. The two kinds of intrinsic transition mix up when \(X_f = 0\). The mass parameter is fixed to be \(\mu c^2 = 2000 MeV\).

The effects of intrinsic degrees of freedom are sensitive to the degree of adiabaticity measured by the adiabaticity parameter \(\lambda = \frac{\hbar}{\Omega}\), \(\omega = \epsilon_2 - \epsilon_1\) and \(\Omega\) being the excitation energy of the intrinsic motion and the curvature of the bare potential barrier \(U(X)\) [3] [3] [3] [3]. We study a fast and slow tunneling represented by \(\lambda = 0.5\) and 2.0, respectively. Since the whole tunneling process crucially depends on the initial condition of the intrinsic motion [14], we discuss both cases where the intrinsic motion is initially in the ground and in the excited states.

Fig.1 compares the barrier transmission probability as a function of the incident kinetic energy calculated in various ways for the case of \(X_f = 50 fm\). The upper and the lower panels correspond to \(\lambda = 0.5\) and 2.0, respectively. They have been calculated by assuming \((a, a_f) = (5 fm, 5 fm)\) and \((15 fm, 5 fm)\),
respectively. In both of them, the thick dashed line is the barrier transmission probability in the absence of the intrinsic motion. As it should, it becomes about 0.5 when the incident energy coincides with the barrier height 10 MeV. The thick solid and the dot-dashed lines have been calculated by direct numerical integration of the coupled-channels equations, i.e. by eq.(18), for the cases where the intrinsic motion starts from the ground and the excited states, respectively. As expected, the barrier transmission probability is hindered over whole energy region by the intrinsic motion if it is initially in the ground state, while it is enhanced if the system starts from the excited state of the intrinsic motion. An interesting observation is that the fast intrinsic motion yields a step-function like structure in the excitation function of the barrier transmission probability, while the barrier transmission probability shows no structure when the macroscopic variable couples with a slow intrinsic degree of freedom.

In order to test the accuracy of the semiclassical mean field theory, the thin solid and the thick dotted lines have been calculated based on eq.(25) for the cases where the intrinsic motion starts from the ground and the excited states, respectively. We observe that the semi-classical mean field theory well reproduces the results of the direct numerical integration of the coupled-channels equations at low energies, though it fails at high energies as a natural consequence of the well known fact that the simple WKB approximation should be replaced by the uniform approximation.

We now consider the case when the coupling form factor is located in the same region as the bare potential barrier by setting \( X_f = 0 \, \text{fm} \). The resultant barrier transmission probability is shown in Fig.2. Similarly to the case of Fig.1, the extension parameters have been chosen to be \((a, a_f) = (5 \, \text{fm}, 5 \, \text{fm})\) and \((15 \, \text{fm}, 5 \, \text{fm})\) for the cases of \( \lambda = 0.5 \) and \( 2.0 \), respectively. The notations are the same as those in Fig.1.

As we discuss in [11], slow intrinsic motion corresponding to \( \lambda = 0.5 \) enhances the barrier transmission probability at low energies and hinders it at high energies irrespective of whether the intrinsic motion is initially in the ground or in the excited states, though quantitative details are different. The fast intrinsic motion, on the other hand, enhances the barrier transmission probability when it starts from the ground state, and hinders when it starts from the excited state for a wide range of the incident energy. Similarly to the previous case when \( X_f = 50.0 \, \text{fm} \), the semiclassical mean filed theory well reproduces the results of the direct numerical integration of the coupled-channels equations at low energies. The accuracy of the semiclassical mean field theory can be more clearly seen in Fig.3, where the barrier transmission probability in low energy region is shown in an expanded scale. This figure is useful also to see that the hindrance effect of a fast intrinsic motion to the barrier transmission probability in the case when it starts from the excited state turns into an enhancement effect at low energies (see the lower panel).

IV. PROPERTIES OF THE INTRINSIC TRANSITION AND THE POTENTIAL RENORMALIZATION

We now discuss the characteristics of the intrinsic transition and the associated potential renormalization. We first consider the case corresponding to Fig. 1, i.e. where the coupling form factor is located at far in front of the barrier region. Fig.4 shows the change of the occupation probability of the ground and the excited states, \( |a(1)|^2 \) (the thick solid line) and \( |a(2)|^2 \) (the thick dotted line), with the position X. The incident direction is toward the negative values of X. Similarly to Fig.1, the upper and lower panels correspond to the cases of coupling to slow or fast intrinsic motion. Each of them is divided into the left and right panels, where the results when the intrinsic state is initially the ground and the excited states, respectively, are shown. The bare potential \( U(X) \) and the coupling form factor \( f(X) \) are also shown in the figure in arbitrary scale. In the tunneling region, \( |a(1)|^2 \) and \( |a(2)|^2 \) have been normalized such that \( |a(1)|^2 + |a(2)|^2 = 1.0 \). The behaviour of \( |a(1)|^2 \) and \( |a(2)|^2 \) as functions of X depends on the incident energy. By considering the accuracy of the semiclassical mean field theory discussed in the previous section, we chose \( E_K \) to be 8.74, 7.64, 9.4 and 6.87 MeV to obtain the upper left, upper right, the lower left and lower right panels, respectively. The semiclassical mean field theory well reproduces the barrier transmission probability obtained by the direct numerical solution of the coupled-channels equations at these energies. In the figure, the short horizontal line in the barrier region indicates the tunneling region.

The behaviour of the occupation probability can be easily understood in the present case. The intrinsic degree of freedom makes transition to the other state from the initial state when the macroscopic motion traverses the coupling region. The interesting result is that it then makes a strong transition to the ground state in the tunneling region even though the coupling form factor is already almost zero in that
We name this the tunneling induced quantum transition of the intrinsic motion, because these transitions take place to increase the tunneling probability.

We now calculate the potential renormalization and the effective potential barrier based on eq. (24) for the classically allowed region and the corresponding expression for the tunneling region. The results are shown in Fig. 5. The input parameters are the same as those for Fig. 4. The figure contains the potential renormalization $\Delta V(X)$ in the case when the intrinsic motion starts from the ground (the solid line) and the excited states (the thick dots), the effective potential $U_{\text{eff}}(X) = U(X) + \Delta V(X)$ for these cases (the dots and the dott-dashed lines). The coupling form factor is also shown (the thin dashed line). We see two different kinds of potential renormalization in Fig. 5. The first is the potential renormalization in the region of the coupling form factor, which one naturally expects to exist. The other is the novel type of potential renormalization that is caused by the tunneling induced intrinsic transition. The important consequence is that the effects of intrinsic motion cannot be represented by a constant potential shift in the tunneling region even though the coupling form factor is outside the tunneling region.

Let us now consider the case when $X_f = 0.0 \text{ fm}$. The resultant position dependence of the occupation probabilities $|a(1)|^2$ and $|a(2)|^2$ and the associated potential renormalization and the net effective potentials are shown in Figs. 6 and 7, respectively. The meaning of each line is the same as that in Figs. 4 and 5. The incident kinetic energy has been chosen to be 6.93, 5.0, 8.96 and 6.43 MeV to obtain the upper left, upper right, the lower left and lower right panels, respectively, in Fig. 6.

Since the two effects, i.e. the transition by the coupling form factor and that induced by the tunneling effect, overlap, the behaviour of $|a(1)|^2$ and $|a(2)|^2$ in the present case gets more complex than the previous case, where the coupling form factor is far outside the tunneling region. The important thing is that the potential renormalization is strongly spatially dependent also in this case. Another interesting observation is that the potential renormalization is larger in the case where the intrinsic motion starts from the excited state than the case when it starts from the ground state. This is related to the choice of the incident energy to draw Fig. 6 and is reflected in the larger enhancement of the barrier transmission probability in the former case as is shown in Fig. 3.

V. SUMMARY

The effect of environmental or intrinsic degrees of freedom on the tunneling probability of a macroscopic variable has been one of the very active subjects in many fields of physics and chemistry in the past decades [12, 13, 14]. One interesting question in this respect is to understand the way the intrinsic degrees of freedom modify the tunneling potential barrier. This question is especially important in connection with low energy nuclear reactions in laboratories, because the large deviation of the experimental reaction rate from the extrapolation from high energy data has been analyzed by assuming a constant potential shift in the tunneling region, which is supposed to well represent the screening effects by bound target electrons, with a puzzling consequence that the obtained screening energy exceeds the theoretically expected upper limit, i.e. the adiabatic limit, for all systems so far studied.

In this paper, we have set a simple two-level coupled-channels problem, and analyzed the properties of the intrinsic transition and the associated potential renormalization by using a semi-classical mean field theory for quantum tunneling, which naturally introduces the concept of the potential renormalization.

One of the main conclusions of our study is that there can occur strong intrinsic transitions in the tunneling region in order to facilitate the quantum tunneling even if there is no coupling any more in that region. We called this phenomenon the tunneling induced or assisted intrinsic transition. We have shown that it leads to a strongly spatially dependent potential renormalization in the tunneling region. This suggests that the screening effects in realistic low energy nuclear reactions should be handled not by simply assuming a constant potential shift as has been done in all previous studies, but by a proper dynamical treatment of the tunneling region. We publish our study in this direction in separate papers [15, 16].

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FIG. 1: The barrier transmission probability as a function of the incident kinetic energy for $X_f = 50 \text{fm}$ calculated in various ways.
FIG. 2: The same as Fig.1, but for $X_f = 0 \text{fm}$.
FIG. 3: The same as Fig. 2, but in an expanded scale.
FIG. 4: The change of the occupation probabilities of the ground and the excited states of the intrinsic motion as functions of the position $X$ for $X_f = 50 fm$ corresponding to the case shown in Fig.1. The incident energy for each of the four panels is given in the text.
FIG. 5: The potential renormalization and the effective potential corresponding to each of the four cases shown in Fig.4.
FIG. 6: The same as Fig. 4, but for $X_f = 0\, fm$ corresponding to Figs. 2 and 3.
FIG. 7: The same as Fig.5, but for $X_f = 0 fm$ corresponding to Fig.6.