Influence of Tunneling on Electron Screening in Low Energy Nuclear Reactions

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Using a semiclassical mean field theory, we show that the screening potential exhibits a characteristic radial variation in the tunneling region in sharp contrast to the assumption of the constant shift in all previous works. Also, we show that the explicit treatment of the tunneling region gives a larger screening energy than that in the conventional approach, which studies the time evolution only in the classical region and estimates the screening energy from the screening potential at the external classical turning point. This modification becomes important if the electronic state is not a single adiabatic state at the external turning point. Furthermore, as an alternative solution of the screening problem, we give the estimation for the effect of extra electrons which are caught into the ground state of the projectile by using constraint molecular dynamics.

§1. Introduction

Nuclear reaction rates at astrophysical energies are interesting quantities for their own sake and also in connection with nucleosynthesis in stars. The bare reaction rates are modified in stars by the screening effects of free and bound electrons. The knowledge of the bare nuclear reaction rates at low energies is important not only for the understanding of various astrophysical nuclear problems, but also for assessing the effects of host material in low energy nuclear fusion reactions in matter.

Rolfs and his colleagues have reported that the experimental cross sections of the ^{3}He$(d,p)^4$He and of D(^{3}He, $p)^4$He reactions with gas target show an increasing enhancement with decreasing bombarding energy with respect to the values obtained by extrapolating from the data at high energies.[1)] Since then similar enhancement has been reported for many systems with not only gas targets, but also with metal targets such as the ^{6}Li$(p,\alpha)^3$He reaction.

These observations have motivated many theoretical as well as experimental studies. Many of them attempted to attribute the enhancement of the reaction rate to the screening effects by bound target electrons. A simple approach is to assume that the screening effects can be well represented by a constant, i.e. radially independent, decrease of the barrier height in the tunneling region. This decrease is named the screening energy. It is determined by making a fit to the data. A puzzle is that the screening energy obtained by this procedure exceeds the value in the so called adiabatic limit, which is given by the difference of the binding energies in the united

atom and in the target atom and is theoretically thought to provide the maximum screening energy, for all systems so far studied experimentally[2] (see Ref. 3) for a recent modification). For $^7\mathrm{Li}(p,\alpha)\alpha$ reaction, in addition to the direct measurement, an indirect measurement of the cross section using the Trojan horse method has recently been made.[4] The comparison between the two methods indicates again that the screening energy in the direct method exceeds the adiabatic limit by a large factor.

In these proceedings, we discuss the properties of the screening potential in the tunneling region. We examine, in particular, whether it can be represented by a constant shift as has been postulated in all previous studies. We also examine the validity of the former dynamical approach in Refs. 5) and 6), which solves the coupled equations for the electronic and nuclear motions only in the classical region, and estimates the screening energy by using the electronic wave function at the external classical turning point. To that end, we describe the time evolution of the electrons by a Schrödinger equation and the relative motion between the projectile and target nuclei by classical Newtonian equations. They are coupled to each other through a variational principle leading to a mean field theory.

One should, however, keep in mind that there are several vague points around the analysis of the screening energy. The stopping power is not well established, especially for gas target, at such low energies.[3),7)–9)] Also different values of the screening energy are obtained depending on the method of analysis.[10),11)] Among these other probable causes, we, in addition, investigate the effect of extra electrons which are caught in a bound state of the projectile especially. It is well known that in the low energy reaction the projectile might catch electrons in the gas target before the fusion. In order to assess this effect, we use the constraint molecular dynamics(CoMD). The advantage of the method is the fact that with CoMD we can treat many-electron systems easier.

§2. Formalism

2.1. *Semiclassical mean field theory of quantum tunneling*

We denote the coordinate of the relative motion between the projectile and target nuclei by $\boldsymbol{R}$ and that of the electrons by ξ, which contains in general the coordinate of the center of mass of electrons relative to the center of mass of the target and projectile nuclei, as well as their intrinsic coordinates. Considering the head on collision, we assume the following Hamiltonian for the total system,

$$H(R,\xi) = -\frac{\hbar^2}{2M}\left[\frac{\partial^2}{\partial R^2} + \frac{2}{R}\frac{\partial}{\partial R}\right] + V^{(0)}(R) + \hat{H}_0(\xi) + V_c(R,\xi), \qquad (2\cdot1)$$

where $V^{(0)}(R)$ is the bare interaction between the target and projectile nuclei, $\hat{H}_0$ is the unperturbed Hamiltonian of the electrons, and $V_c(R,\xi)$ is the interaction between the electrons and nuclei. Denoting the wave function of electrons and the distance between the projectile and the target at time t by $\phi(\xi,t)$ and $R(t)$, respectively, the time dependent Schrödinger equation and the classical Newtonian equation for them

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$$i\hbar\frac{\partial\phi(\xi,t)}{\partial t} = \left[H_0(\xi) + V_c(R(t),\xi)\right]\phi(\xi,t), \tag{2·2}$$

$$M\frac{d^2R(t)}{dt^2} = -\frac{d}{dR}\left[V^{(0)}(R) + \Delta V(R)\right], \tag{2·3}$$

where

$$\Delta V(R) = \langle\phi|\left[H_0(\xi) + V_c(R(t),\xi)\right]|\phi\rangle. \tag{2·4}$$

Equations (2·2) and (2·3) lead to the following energy conservation law.

$$\frac{M}{2}\left(\frac{dR(t)}{dt}\right)^2 + V^{(0)}(R(t)) + \Delta V(R) = E. \tag{2·5}$$

We determine the time evolution in the classically allowed region by solving Eqs. (2·2) and (2·3) along the real time axis with the proper initial condition. Once the velocity of the relative motion becomes zero, we switch to the imaginary time, $t = -i\tau$, and continue to follow the time evolution in the tunneling region using the following equations,

$$\hbar\frac{\partial\phi(\xi,\tau)}{\partial\tau} = -\left[H_0(\xi) + V_c(R(\tau),\xi)\right]\phi(\xi,\tau), \tag{2·6}$$

$$M\frac{\partial^2R(\tau)}{\partial\tau^2} = \frac{\partial}{\partial R}\left[V^{(0)}(R) + \Delta V(R)\right]. \tag{2·7}$$

The screening potential and the energy conservation law in the tunneling region are given by

$$\Delta V(R) = \frac{\langle\phi|\left[H_0(\xi) + V_c(R(\tau),\xi)\right]|\phi\rangle}{\langle\phi|\phi\rangle}, \tag{2·8}$$

$$-\frac{M}{2}\left(\frac{\partial R(\tau)}{\partial\tau}\right)^2 + V^{(0)}(R(\tau)) + \Delta V(R) = E. \tag{2·9}$$

We note that the norm of the wave function of electrons is not conserved in the tunneling region. Accordingly, the denominator of the screening potential given by the r.h.s. of Eq. (2·8) is essential as we see later. We note also that the potential renormalization given by Eq. (2·8) is the equivalent potential of the dynamical norm factor, which has been introduced in Ref. 12) in order to take non-adiabatic effects into account to correct the calculation of the tunneling probability in the adiabatic approximation.

Using the screening potential in the tunneling region thus obtained, we calculate the tunneling probability in the presence of electrons by the following WKB formula

$$\begin{aligned} P(E) &= \exp\left(-2\sqrt{\frac{2M}{\hbar^2}}\int_{R_b}^{R_a} dR\sqrt{V^{(0)}(R) + \Delta V(R) - E}\right) \\ &= \exp\left(\frac{-4}{\hbar}\int_{\tau_a}^{\tau_b} d\tau[V^{(0)}(R) - E]\right)\exp\left(\frac{-4}{\hbar}\int_{\tau_a}^{\tau_b} d\tau\Delta V(R)\right), \end{aligned} \tag{2·10}$$

where R_a and R_b are the classical turning points on both sides of the effective potential barrier $V^{(0)}(R) + \Delta V(R)$, and τ_a and τ_b are the corresponding times along the imaginary time axis. We then convert the enhancement factor

$$f = P(E)/P_0(E'), \tag{2·11}$$

where $P_0(E')$ is the tunneling probability in the absence of electrons, into a screening energy using the relation

$$U_e = \frac{E_K^\infty}{\pi\eta(E_K^\infty)} \log\left(\frac{P(E)}{P_0(E')}\right) = \frac{E_K^\infty}{\pi\eta(E_K^\infty)} \log\left(\frac{P(E_K^\infty + \epsilon^{(i)})}{P_0(E_K^\infty)}\right), \tag{2·12}$$

where $\eta(E)$ is the Sommerfeld parameter, E_K^∞ is the kinetic energy of the relative motion between the target and projectile nuclei and $\epsilon^{(i)}$ is the total energy of electrons in the center of mass system in the initial asymptotic region. The latter is identical with the screening potential ΔV at the initial time and is given by

$$\epsilon^{(i)} = \frac{1}{2}\mu_e v_T^2 + \epsilon_T, \tag{2·13}$$

where ϵ_T is the binding energy of electrons in the initial state in the target atom and $v_T = \frac{M_P}{M_T+M_P} v_\infty$, v_∞ being $\frac{\partial R(t)}{\partial t}$ at $t = -\infty$, is the velocity of the target nucleus relative to the center-of-mass of the projectile and target nuclei at the initial time. The reduced mass μ_e is given by $\frac{1}{\mu_e} = \frac{1}{m_e} + \frac{1}{M_T+M_P}$. Note that we compare the tunneling probabilities for the same kinetic energy of relative motion of the nuclei in the presence and in the absence of the electrons. That is why we use different notations for the energy arguments in the barrier penetrability in the second term of Eq. (2·12). Also, we use in Eq. (2·12) and in what follows the lower index 0 to denote the barrier penetrability and the cross section calculated in a two body system and distinguish them from the corresponding quantities calculated including electrons.

2.2. *Constraint molecular dynamics*

The formalism of this method is described in Ref. 13). In this method we use classical equation of motion for the electrons as well, instead of the wave function in the semiclassical mean field theory. We take into account the behavior of the wave function, considering many events and taking average. In order to make the bound state of the electrons around the target and projectile nuclei, we use constraints which satisfy the Heisenberg uncertainty principle and the Pauli exclusion principle. In this method the enhancement factor is given by Eq. (2·11) for each event, replacing $\Delta V(R)$ by the energy of the electrons.

§3. Applications

3.1. *D+d reaction*

We now apply our formalism to D+d reaction. We choose these systems for simplicity of the treatment because the screening effects are due to a single electron. Moreover, there exists experimental data for the D+d reaction[14] at a low energy, i.e.

at $E_{\rm cm}$= 1.62 keV, though experiments have been performed for a molecular target rather than an atomic target.[14] Figure 1 shows the screening potential for the D+d reaction at $E_{\rm cm}$=1 keV (solid line) and 200 keV (dashed line). The asymptotic values and their incident energy dependence can be understood from Eq. (2·13). The closed triangles show the external classical turning points.

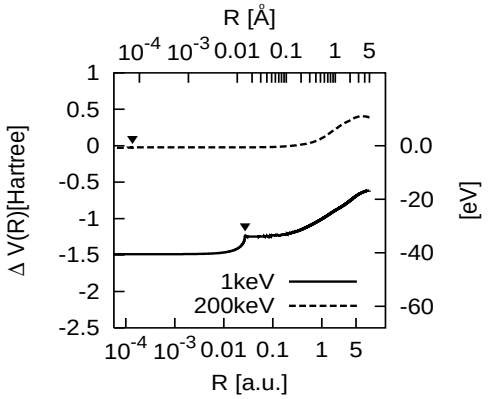

Fig. 1. Screening potential for the D+d reaction at the center-of-mass energies 1 and 200 keV as a function of the separation distance between the nuclei. The filled triangles show the position of the external classical turning point.

Two interesting things can be noticed. The first is that the value of the screening potential at the external turning point for 1 keV is −34.0 eV, which matches with the average of binding energies $\epsilon_{UA}^{(g)}$=−54.4 eV in the lowest gerade and $\epsilon_{UA}^{(u)}$=−13.6 eV in the ungerade states, i.e. in the 1s- and 2p-states, of the united atom $^4He^+$. This indicates that the reaction takes place almost adiabatically in both gerade and ungerade configurations at this energy. The second observation is that the screening potential for $E_{\rm cm}$ = 1 keV changes very fast just inside the external classical turning point. This can be understood from Eqs. (2·8) and (2·6) as a consequence that the contribution to the mean potential from the ungerade configuration, which has higher electronic energy, quickly dies out as the relative motion between the projectile and target penetrates into the tunneling region. In the case for D+d reaction, where the symmetry of the system admixes the gerade and ungerade states with equal weight at any incident energies including the low energy adiabatic limit.

Figure 2 shows the screening energy for the D+d reaction. The closed circles are the results of our method. The open squares have been calculated in the same way as in Ref. 5). The horizontal solid and dashed lines are the screening energies in the sudden and adiabatic reaction limits, $U_e^{(S)}$ and $U_e^{(AD)}$, respectively, which are given by

$$U_e^{(S)} = \frac{M_T}{M_P + M_T} \times 2 \times Z_P Z_T \times \epsilon_H, \tag{3·1}$$

$$= 13.6 \text{ eV}, \tag{3·2}$$

$$U_e^{(AD)} = \epsilon_T - \epsilon_{UA} \tag{3·3}$$

$$= \frac{1}{2}\left[(54.4 - 13.6) + (13.6 - 13.6)\right] \text{ eV} \tag{3·4}$$

$$= 20.4 \text{ eV}. \tag{3·5}$$

Equation (3·1) has assumed that the screening electron occupies the 1s state of the target atom. In Eq. (3·1), $\epsilon_H = 13.6$ eV is the binding energy of the 1s orbit in the Hydrogen atom. In Eq. (3·3), ϵ_T and ϵ_{UA} are the binding energies of the electron in the

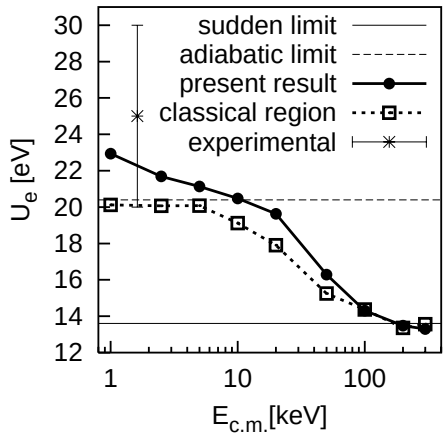

Fig. 2. Screening energy U_e as a function of the incident center-of-mass energy for the D+d reaction. The experimental value is for a molecular deuteron target taken from Ref. 14).

target and united atoms, respectively. The electron is assumed to occupy the adiabatic state with the same label i in both atoms because of the slow adiabatic process. In the second line of $U_e^{(AD)}$, i.e. in Eq. (3·4), we have used the actual values in the present case by taking the symmetry property of the D+d system into account. As one expects, the screening energy converges to that in the sudden reaction limit at high energies. It converges to the adiabatic limit at low energies if one calculates in the way of Ref. 5) by studying only the classical region. The star with error bar is the experimental value taken from Ref. 14). However, this should be taken merely as a reference, because as mentioned before the experiments have been performed not for an atomic deuteron target, but for a molecular deuteron target.

The remarkable thing is that our calculations give systematically a larger screening energy than that in the conventional calculations. At low energies, this can be understood in the following way. Using the screening potential at the external turning point R_t, the enhancement factor is calculated in the conventional method, e.g. in Ref. 5), by

$$f_c = \frac{\sigma_0(E_K^\infty + \epsilon^{(i)} - \Delta V(R_t))}{\sigma_0(E_K^\infty)} \tag{3·6}$$

$$\approx \frac{\sigma_0(E_K^\infty + \epsilon_T - \Delta V(R_t))}{\sigma_0(E_K^\infty)} \tag{3·7}$$

$$\approx \frac{\sigma_0(E_K^\infty + (U_e^{(g)} + U_e^{(u)})/2)}{\sigma_0(E_K^\infty)}. \tag{3·8}$$

In transforming from Eq. (3·6) to Eq. (3·7), we have ignored the difference between $\epsilon^{(i)}$ and ϵ_T given by Eq. (2·13) in accord with the adiabatic process. Also, in order to move further to Eq. (3·8), we have used the fact, which we remarked before concerning Fig. 1, that the screening potential at the external classical turning point can be understood in terms of the binding energies of the electron in the gerade and ungerade configurations of the united atom. On the other hand, our method, which handles the tunneling region explicitly, leads to

$$f_t = \frac{\sigma^{(g)} + \sigma^{(u)}}{2\sigma_0} \tag{3·9}$$

$$= \frac{\sigma_0(E_K^\infty + U_e^{(g)}) + \sigma_0(E_K^\infty + U_e^{(u)})}{2\sigma_0(E_K^\infty)} \tag{3·10}$$

for the enhancement factor. These equations can be derived from Eqs. (2·6), (2·8) and (2·10) by assuming that there are no change with the adiabatic energies and the adiabatic states in the tunneling region. Since the excitation function of the fusion cross section is a convex increasing function of the incident energy, f_t is larger than f_c. The conventional method thus underestimates the screening energy.

Figure 2 clearly exemplifies this effect. It is important to properly calculate the enhancement factor in order to get a reliable value of the screening energy. This can be achieved either by explicitly handling the tunneling region like in our method, or by studying the distribution of the electronic state over different adiabatic states at the external classical turning point, and calculate the fusion probability for each of them and taking average afterwards with the proper weight. This fact can be generalized for the reactions which involve many adiabatic states.[15)]

3.2. *^{3}He+d and ^{3}He+D reaction*

These effects which we mentioned above are, however, too small to explain the large experimental screening energies for almost all systems reported in Ref. 2). In this connection, the large screening energy obtained in this study for the D+d reaction has been caused by the symmetry special to this system, and cannot be generalized to other systems. Figure 3 shows the incident energy dependence of the screening energy U_e for the ^{3}He+d reaction, i.e. we assume the ground state of an atomic helium, with two electrons as the target and a deuteron as the projectile. The experimental value is taken from Ref. 16). In Fig. 3 it is clear that neither the results which is obtained by studying only the classical region(CT, open squares) nor our results(SCMFQT, filled circles) exceed the adiabatic limit. It is due to the fact that the electrons occupy the ground state of the total system in the initial asymptotic region. Consequently the electrons occupy the lowest state at the classical turning point, in the case where the incident energy is enough low. Among the other many probable causes, like the determination of the stopping power, as we referred to before, here we mention the capture of electrons by the projectile especially. It is well known that the projectile, in this case deuteron, might catch electrons in the gas target before the fusion with the target. In order to estimate the effect of this extra electron, we use the constrained molecular dynamics(CoMD), with which we can treat the

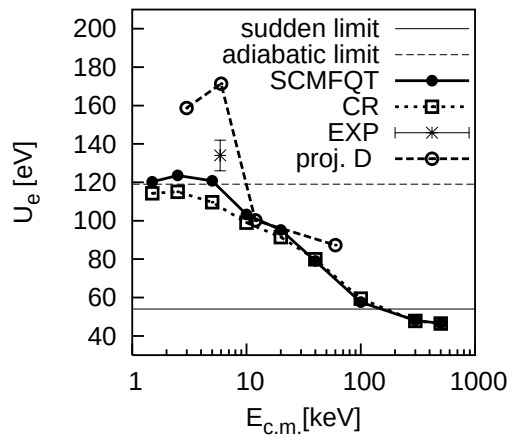

Fig. 3. The same as Fig. 2, but for the ^{3}He+d reaction and the ^{3}He+D reaction (only open circles)

system with many electrons easier. The CoMD is a method to treat quantum-mechanical systems.

In Fig. 3 the open circles show the screening energy of the ^{3}He+D reaction. The results are still preliminary but gives systematically larger screening energies than that of the ^{3}He+d case.

§4. Summary

We have presented a semiclassical mean field theory of quantum tunneling which treats both classical and tunneling regions in a consistent way. Applying the formalism to the problem of screening effects by bound target electrons in low energy nuclear reactions in laboratories, we have shown that the screening potential shows a characteristic radial variation contrary to the assumption of a constant potential shift in all previous analyses. We have shown also that the proper treatment of the tunneling region leads to an increase of the screening energy compared with that estimated in the previous mean field theory, which studies only the classical region and calculates the tunneling probability by using the average potential at the external classical turning point. The above effects are, however, too small to explain the large experimental screening energies reported in Ref. 2). Remember in this connection that the large screening energy obtained in this study for the D+d reaction has been caused by the symmetry special to this system, and cannot be generalized to other systems. As a candidate of alternative solution, we examined the effect of the extra electrons bounded by projectile using the constraint molecular dynamics for the ^{3}He+D reaction.

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