Abstract

We calculate the electron screening effect in low energy nuclear fusion reactions by taking non-adiabaticity of the tunneling process into account. In order to investigate deviations from the adiabatic limit, we use the dynamical norm method, which has recently been developed by the present authors. Using $d+D$ reaction as an example, we show that the screening energy never exceeds those estimated in the adiabatic approximation. Our calculations indicate that the non-adiabatic effect is important both in classically allowed and classically forbidden processes.

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Nuclear reactions at very low energies are important for several problems of nuclear astrophysics. An interesting problem is whether they are significantly affected by bound or free electrons when the reactions take place in laboratory experiments or in condensed matters. The screening effects by bound electrons in laboratory experiments have been reported indeed in ref.[1–8]. In these experiments, the target is in the form of a neutral atom or molecule. The electron clouds surrounding the target nucleus screen the Coulomb repulsive potential between the colliding nuclei. Consequently, the Coulomb barrier is reduced. This leads to an enhancement of the fusion cross section and the corresponding astrophysical $S$ factor. This effect becomes significant at very low bombarding energies. At such energies, the penetrability through the Coulomb barrier exponentially decreases with decreasing bombarding energy. The barrier penetrability is, therefore, very sensitive to an even tiny change of the potential barrier of the order of electron volt due to the screening effects of the bound electrons.

Shoppa et al. studied the shift of the Coulomb barrier due to the electron screening by solving the wave functions for electrons in the classically allowed region. In contrast to static estimates of the screening effects in either the adiabatic or sudden approximations, they investigated the incident energy dependence of the screening effect[5]. Their calculations clearly show the transition from the adiabatic to the sudden limits with increasing bombarding energy, and suggest the importance of non-adiabatic effects at intermediate energies between the two extreme limits.

However, they do not explicitly handle the tunneling process. They assumed a constant energy shift inside the tunneling region once they estimated it at the classical turning point. In this paper we explicitly treat the tunneling process and investigate the non-adiabatic effects in the electron screening. To this end, we use the dynamical norm method[9], which can be applied to wide range of problems of quantum tunneling in
systems with many degrees of freedom lying between the adiabatic and sudden tunneling limits [10]. This method first uses the tunneling probability in the adiabatic limit as the reference. The effects of deviation from that limit is then taken into account through the reduction of the norm of the environmental space during the classically forbidden process.

Our interest is to calculate the tunneling rate of the relative motion between the colliding nuclei in the presence of electronic degrees of freedom. In particularly we consider in this paper the reaction between deuterons($d$) and deuterium atoms(D), for which experimental data on the possible effects of the electron screening have recently been reported[6]. Moreover, this system is easier to be handled because it contains only one electron, though the dynamical norm method can be easily extended to study more complex systems such as the experimentally well studied $d+^3$He system, where there exist two bound electrons.

In the problem of electron screening, one often represents the enhancement of the cross section in terms of the so called screening energy $U_e$ defined by

$$U_e = \frac{E}{\pi \eta(E)} \log f$$

where $f$ is the enhancement factor of the cross section i.e., the ratio of the cross section to that estimated for the bare Coulomb barrier. The bombarding energy in the center of mass frame and the Sommerfeld parameter are denoted by $E$ and $\eta(E)$, respectively. Equation (1) corresponds to assuming that the electron clouds provide a constant energy shift $U_e$ of the Coulomb barrier[3]. In the adiabatic tunneling limit, the screening energy is given by the difference in atomic binding energies between the compound nucleus and the entrance channel[7]. For $d+D$ reactions, the electron occupies the equally weighted linear combination of the lowest energy gerade and ungerade molecular orbitals in the entrance channel[11]. Therefore, the screening energy in the adiabatic approximation reads

$$U_{ad} = \frac{E}{\pi \eta(E)} \log \left[ \frac{1}{2} \left\{ \exp \left( \pi \eta(E) \frac{\Delta E_g}{E} \right) + \exp \left( \pi \eta(E) \frac{\Delta E_u}{E} \right) \right\} \right]$$
where $\Delta E_g = 40.7$ eV is the difference of the binding energy of electron in the 1s orbitals of He$^+$ atom and of D, whereas $\Delta E_u = 0$ eV that in the 1p orbital of He$^+$ atom and in the 1s orbital of D [7]. Note that the adiabatic screening energy $U_{ad}$ has the bombarding energy dependence. This is a characteristic feature of the system with two identical nuclei.

After discarding the center of mass motion of the whole system, we choose the internuclear separation $R$ and the electron center of mass location $r$, which is measured from the center of mass of the two nuclei, as two independent coordinates. The Hamiltonian then reads

$$ H = -\frac{\hbar^2}{2\mu} \nabla_R^2 - \frac{\hbar^2}{2m_e} \nabla_r^2 + \frac{e^2}{R} - \frac{e^2}{|r + \frac{R}{2}|} - \frac{e^2}{|r - \frac{R}{2}|} \quad (3) $$

where $\mu$ and $m_e$ is the reduced mass between deuterons and the electron mass, respectively.

The time dependent Schrödinger equation for the electron in the external Coulomb field generated by two moving deuterons is given by

$$ i\hbar \frac{\partial}{\partial t} \psi(r, t) = \left( -\frac{\hbar^2}{2m_e} \nabla_r^2 - \frac{e^2}{|r + \frac{R(t)}{2}|} - \frac{e^2}{|r - \frac{R(t)}{2}|} + U_{ad} \right) \psi(r, t) \quad (4) $$

Following ref. [9], we subtract the adiabatic screening energy $U_{ad}$ from the potential energy of the relative motion between deuterons and add it to the electronic Hamiltonian.

The initial wave function for the electron $\psi(r, t = 0)$ is the ground state of the deuterium atom boosted to the correct center of mass velocity. We assume that the electronic wave function is azimuthally symmetric about the collision axis[5]. We use the method in ref.[12] to perform the time integration. This method modifies the Peaceman-Rachford method [13, 14] by incorporating with the time expansion up to the second order of the time step of the integration.

We solve eq.(4) from the initial position of $R$, which we choose to be 10 a.u., to the outer classical turning point by assuming that the relative distance between two deuterons
\( R(t) \) obeys
\[
\frac{\partial R}{\partial t} = -\sqrt{\frac{2}{\mu}} \left( E - \frac{e^2}{R} - U_{ad} \right)
\]
(5)

At the outer turning point, we switch the time to imaginary \((it \rightarrow \tau)\) and solve the time dependent Schrödinger equation along the imaginary time axis
\[
-\hbar \frac{\partial}{\partial \tau} \psi(r, \tau) = \left( -\frac{\hbar^2}{2m_e} \nabla_r^2 - \frac{e^2}{|r + R(\tau)|} - \frac{e^2}{|r - R(\tau)|} + U_{ad} \right) \psi(r, \tau)
\]
(6)

with
\[
\frac{\partial R}{\partial \tau} = -\sqrt{\frac{2}{\mu}} \left( \frac{e^2}{R} - U_{ad} - E \right)
\]
(7)

We solve these equations up to the inner turning point, which we assume to be twice of the deuteron radius. Note that eq.(6) describing the time evolution of the electronic wave function does not conserve the norm of the wave function. Following the dynamical norm method, the tunneling probability for the inclusive process is given by
\[
P(E) = P(E + U_{ad}) \cdot N,
\]
where \( N \) is the norm of the electronic wave function at the inner turning point\[9\]. The enhancement factor is then given by
\[
f = f_{ad} \cdot N = \exp \left( \pi \eta(E) \frac{U_{ad}}{E} \right) \cdot N
\]
(8)

The dynamical norm factor \( N \) represents the deviation from the adiabatic tunneling limit.

Figure 1 shows the enhancement factor of the barrier penetrability as a function of the bombarding energy. The solid line is the result of the dynamical norm method (see eq.(8)), while the dotted line is that in the adiabatic approximation. Over the whole range of the bombarding energy shown in this figure, the adiabatic approximation overestimates the enhancement factor. As we have remarked in refs.\[4, 15\], the adiabatic approximation gives the upper bound of the tunneling rate.

Figure 2 shows the screening energy obtained from the enhancement factor according to eq.(1). The meaning of the solid and the dotted lines is the same as in fig.1. The
dashed line corresponds to the result reported in ref.[5], where the screening energy was estimated by studying the electronic wave function only in the classically allowed region. In all calculations, the screening energy decreases as the bombarding energy increases. The large difference between the dotted and the solid lines show that the non-adiabatic effect is significant in the tunneling region. Further, we notice that the dynamical norm method (the solid line) gives a significantly smaller screening energy than that in ref.[5] (the dashed line). This indicates that one needs to properly treat the tunneling region in order to correctly estimate the screening energy.

In summary, we discussed the non-adiabatic effect in the problem of the electron screening in fusion reaction at low energies. Comparison with the results in ref.[5] shows that the non-adiabatic effects are important both in classically allowed and in classically forbidden processes. We showed that the screening energy decreases with increasing bombarding energy. An unsolved puzzling problem in this field is that experimentally observed screening effect is significantly larger than that estimated in the adiabatic approximation[1, 8]. We showed that the non-adiabatic effects further reduce the tunneling rate estimated in the adiabatic approximation. Therefore the experimental enhancement of the fusion cross section at extremely low energies in $d + D$ and other systems, where large enhancement of the fusion cross section at low energies have been reported like $d + ^3He$, might require additional ingredients to the electron screening. A possible candidate is the polarization of the colliding deuteron[17]. This problem will be reported in a separate paper.

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Figure Captions

FIG.1: Enhancement factor of the barrier penetrability as a function of the bombarding energy for $d+D$ reaction. The solid line is the result of the dynamical norm method, which takes the reduction of the tunneling rate due to the non-adiabatic effect into account. The dotted line was obtained by using the adiabatic approximation.

FIG.2: Screening energy defined by eq. (1) as a function of the bombarding energy. The meaning of the solid and the dotted lines is the same as in fig.1. The dashed line was obtained by the same approach as in ref. [5]. The solid line explicitly treats the dynamics in the tunneling region, while the dashed line was obtained by studying the wave function of the electron only in the classically allowed region.
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