Influence of electron capture and Coulomb explosion on electron screening in low energy nuclear reactions in laboratories

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Abstract

We discuss the effects of electron capture by the projectile and the Coulomb explosion of a molecular projectile on the electron screening in low energy nuclear reactions in laboratory. Using the idea of equilibrium charge, we show that the electron capture of projectile leads to a screening energy which significantly exceeds the adiabatic limit in the simple consideration for the D(d,p)T reaction and provides a possibility to explain the large screening energy claimed in the analysis of experimental data. We then show that the Coulomb explosion can result in a large apparent screening energy as large as that encountered in the analysis of $^3$He(d,p)$^4$He reactions induced by the molecular $D_2^+$ and $D_3^+$ projectiles at very low energies.

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I. INTRODUCTION

Nuclear reaction rates at the Gamow energy play a key role in the synthesis of elements and generation of energy in stars. However, it is difficult to determine them directly by experiments in laboratories because of the small cross section due to the tunneling procedure through the Coulomb barrier. One then tries to determine them by extrapolating the reaction rates observed at high energies to lower energies. The extrapolation is usually done for the astrophysical $S(E)$ factor introduced by

\[ \sigma(E) = \frac{S(E)}{E} \exp(-2\pi\eta) \]  

(1)

with the Sommerfeld parameter $\eta = \frac{Z_1 Z_2 e^2}{\hbar v}$, $Z_1$ and $Z_2$ being the atomic numbers of the projectile and target nuclei and $v$ the initial velocity of the collision, and assuming that $S(E)$ depends only weakly on energy and can be well parametrized with a low order polynomial unless resonance states are involved.

As the measurements are extended to lower energies, the observed values have been found to be significantly larger than those predicted by the extrapolation of the cross section at high energies [1]. The enhancement gets larger with decreasing collision energy. Many works have been reported which try to attribute this phenomenon to the screening effect by bound electrons in the target and in some cases also in the projectile. Assuming that the screening effect can be well represented by a spatially constant lowering of the Coulomb barrier by the amount of $U_e$, one often expresses the enhancement of the cross section by

\[ f \equiv \frac{\sigma(E)}{\sigma_0(E)} = \frac{\sigma_0(E + U_e)}{\sigma_0(E)} = \frac{S(E + U_e)}{S(E + U_e)} \exp[-2\pi\eta(E + U_e)] \exp[-2\pi\eta(E)] \approx \exp\left\{ \frac{\pi\eta(E) U_e}{E} \right\}. \]  

(2)

Here, $\sigma(E)$ and $\sigma_0(E)$ are the true cross section and the cross section in the absence of screening effects, respectively. It was assumed that $U_e \ll E$ and $S(E)$ is almost energy independent. The $U_e$ is called the screening energy.

A puzzle is that the value of screening energy which was determined by fitting the experimental data with eq. (2) exceeds the theoretical value in the so called adiabatic limit, which is given by the difference of the binding energies of electrons in the united atom and in the
initial state in the target or projectile and is thought to provide the maximum screening energy, for all systems so far studied experimentally [2]. In a recent paper [3] one of the authors of the present paper has discussed the influence of tunneling on electron screening and pointed out that the electron screening can exceed the adiabatic limit if the electronic state is not a single adiabatic state at the external turning point either by pre-tunneling transitions of the electronic state or by the symmetry of the system. However, the amount of excess is negligibly small to explain the large experimental value of the screening energy. Alternatively, the stopping power at low energies [4, 5, 6] and also the values of the screening energy [7, 8] have recently been reexamined.

In this paper we reexamine the effects of electron capture by the projectile and of the Coulomb explosion which seem to have been omitted in most recent works since the pioneering works [9] and [10], respectively. In Sect. II, we collect a few basic formulae for the screening energy. In Sects. III and IV we discuss the effects of electron capture and the Coulomb explosion, respectively. We summarize the paper in Sect. V.

II. SCREENING ENERGY IN THE PRESENCE OF ADMIXTURE OF ADIABATIC STATES

The Coulomb explosion leads to a spread in the energy of the nuclear reaction, while the electron capture to an admixture of electronic states. Denoting the screening energy in the n-th state and the corresponding mixing probability as $U_e^{(n)}$ and $P_n$, respectively, we evaluate the net enhancement factor by

$$f = \frac{\sum P_n \times \sigma_0(E + U_e^{(n)})}{\sigma_0(E)}. \quad (3)$$

It is then converted into the screening energy by

$$U_e = \frac{E}{\pi \eta(E)} \log \sum_n \left[ P_n \exp \left\{ \pi \eta(E) \frac{U_e^{(n)}}{E} \right\} \right]. \quad (4)$$

We note that the screening energy estimated by eq. (4) is larger than a simpler estimate, where the enhancement factor is evaluated as

$$f = \frac{\sigma_0(E + \sum P_n \times U_e^{(n)})}{\sigma_0(E)}. \quad (5)$$
and consequently the screening energy is given by

\[ U_e = \sum_n P_n U_e^{(n)}. \]  

(6)

Eqs. (5) and (6) ignore the variation of the tunneling probability in each channel [3].

III. EFFECTS OF ELECTRON CAPTURE

We first discuss the effect of electron capture by the projectile. The charge state of the projectile can be different from the initial one at the time when it reacts with the target. This effect will become increasingly important as the energy gets lower. It is related to the fact that the stopping power of a charged particle passing through matter originates mainly from the exchange of electrons between the incoming charged particle and the surroundings in some low energy region [6, 11]. One could thus use a similar technique in order to study the role of electron capture in the screening problem. For example, a simple estimate of the probability of the electron capture by the projectile and the charge exchange between the projectile and the target material could be obtained by solving the time evolution of the system consisting of the incident ion and a neutral target with a single valence electron. It suggests a large probability of electron capture by the projectile at low energies [6, 12]. In this paper, we resort to the idea of the equilibrium charge [13] in order to estimate the average charge state of the projectile when it reacts with the target.

Let us consider D(d,p)T reaction at \( E = 1.62 \text{ keV} \), which is the lowest energy where experimental measurements were ever performed, as the first example. According to [13], the incoming deuteron captures an electron to become a neutral deuterium atom D in the probability of about 90 % and remains to be deuteron in only 10 % probability at this energy. In the latter case, eq. (4) gives the screening energy to be \( U_e = 22.0 \text{ eV} \) by taking the admixture of the gerade and ungerade configurations with equal weight due to the symmetry of the system into account [3]. In order to evaluate the screening energy for the former, i.e. for the D+D reaction, we notice that the whole colliding system will converge to the ground and to the first excited states of He atom in the adiabatic limit with the probability of 1/4 and 3/4, respectively, reflecting the statistical weights of the total spin of the two electrons. Referring to [14, 15] for the binding energy of electrons, the screening energy in each charge
state is given by,

\[ 78.9 - (13.6 + 13.6) = 51.7 \text{[eV]} \quad \text{(ground state)} \]
\[ 59.1 - (13.6 + 13.6) = 31.9 \text{[eV]} \quad \text{(first excited state)} \]

Eq. (4) then leads to the screening energy \( U_e = 37.1 \text{eV} \) for this channel at \( E = 1.62 \text{keV} \). The net screening energy, which is observed experimentally, should be given by the average of these two charge states with the weights of 1:9. Using eq. (4), we finally obtain \( U_e^{(c)} = 35.7 \text{eV} \), where the upper suffix \( (c) \) stands for capture of electrons by the projectile.

The second example of the effect of electron capture by the projectile is the \(^3\text{He}(d,p)^4\text{He}\) reaction at \( E = 5.01 \text{keV} \). In this reaction, about \( 10 \sim 20\% \) of the projectile captures an electron. The D and d projectile lead to the ground states of Li and Li\(^+\), respectively. The screening energy for each case is

\[ 203.4 - (78.9 + 13.6) = 110.9 \text{[eV]} \quad \text{(D + } ^3\text{He)} \]
\[ 198.0 - 78.9 \quad = 119.1 \text{[eV]} \quad \text{(d + } ^3\text{He)} \]

in the adiabatic limit. If we assume the ratio of the D to d projectile to be 2 to 8, \( U_e^{(c)} = 117.5 \text{eV} \) is obtained for \( E = 5.01 \text{keV} \) as the effective screening energy. The third example is \( D(^3\text{He},p)^4\text{He} \) reaction at \( E = 4.22 \text{keV} \), where the projectile is expected to change into a neutral He in about \( 85\% \) and He\(^+\) in the remaining \( 15\% \) in the state of equilibrium charge at low energies. In the case of \(^3\text{He} + \text{D}\), the system converges to the ground state of Li, while in the case of \(^3\text{He}^+ + \text{D}\), the system will go into the triplet state of Li\(^+(1s)(2s)\) in the probability \( 3/4 \) and to the singlet state in the \( 1/4 \) probability \([9, 16]\). If the screening energies in each state,

\[ 203.4 - (78.9 + 13.6) = 110.9 \text{[eV]} \quad (^3\text{He + D}) \]
\[ 137.2 - (54.4 + 13.6) = 69.2 \text{[eV]} \quad (^3\text{He}^+ + \text{D, singlet}) \]
\[ 139.1 - (54.4 + 13.6) = 71.1 \text{[eV]} \quad (^3\text{He}^+ + \text{D, triplet}), \]

are averaged with the ratio, \( ^3\text{He} + \text{D} : ^3\text{He}^+ + \text{D} = 8.5 : 1.5 \), the effective screening energy \( U_e^{(c)} = 105.3 \text{eV} \) is obtained for \( E = 4.22 \text{keV} \).

**TABLE I** compares the effective screening energy \( U_e^{(c)} \) which takes the effect of electron capture into account, the screening energy \( U_e \) estimated by ignoring electron capture, and
TABLE I: Comparison of the screening energy estimated by taking electron capture by the projectile into account $U_e^{(c)}$, that estimated by ignoring it $U_e$ and the experimental value $U_{e}^{exp}$.

| Reaction          | $E_{min}$ (keV) | $U_e$ (eV) | $U_e^{(c)}$ (eV) | $U_{e}^{exp}$ (eV) |
|-------------------|-----------------|------------|-----------------|------------------|
| D(d,p)T           | 1.62            | 22.0       | 35.7            | 25 ± 5 [17]      |
| $^3$He(d,p)$^4$He | 5.01            | 119.1      | 117.5           | 219 ± 7 [18]     |
| D($^3$He,p)$^4$He | 4.22            | 70.6       | 105.3           | 109 ± 9 [18]     |

the experimental data $U_{e}^{exp}$ [17, 18]. All the theoretical values were estimated by assuming adiabatic limit as described in the preceding paragraphs. The lower index $min$ in $E_{min}$ indicates that it is the lowest center-of-mass energy where experiments have so far been performed. The table shows that the electron capture reduces the screening energy for the $^3$He(d,p)$^4$He reaction. This is caused because the energy level of the captured electron is higher in the united atom than in the initial atom. As ref. [19] concluded, the observed large screening energy in this system cannot be accounted for by the electron screening alone.

To the contrary, the electron capture increases the screening energy for the D(d,p)T and D($^3$He,p)$^4$He reactions. For these reactions, the effective screening energy $U_e^{(c)}$, which includes the effects of electron capture, is as large as the experimental value $U_{e}^{exp}$ or even larger. In comparison, however, one should note that experiments are done using a molecular target, while our calculations were performed by approximating the molecule by the atom. Shoppa et al. [19] showed that the screening effect strongly depends on the molecular orientation and that the screening energy for a molecular target is smaller in general than that for an atomic target unless a counter effect such as the reflection symmetry for the D(d,t)T reaction exists. In our case, the effective beam is the admixture of the original deuteron beam and the deuterium beam after electron capture. The screening energy in the actual molecular target will be larger for the deuteron beam than that estimated for the atomic target, while it will be smaller for the deuterium beam. One should modify the effective screening energy $U_e^{(c)}$ shown in TABLE I by taking these counter effects into account in order to compare with the experimental value.
IV. EFFECTS OF COULOMB EXPLOSION

We now discuss the influence of Coulomb explosion on the observed screening energy in the \(^3\text{He}(d,p)^4\text{He}\) reaction when experiments are carried out with diatomic \((^2\text{D}^+\text{He})\) or triatomic \((^3\text{D}^+\text{He})\) beams instead of an atomic deuteron beam \((^1\text{D}^+\text{He})\). This is the case in [18] at ultra-low energies.

We assume that the electron in the molecular beam is quickly lost in the target material and leads to the Coulomb explosion. We assume that the loss of electron occurs by the exchange process in the opposite direction of the electron capture by the projectile discussed in the previous section and assume that the electron is transferred dominantly to the state with a similar binding energy as that in the original molecule. In a simple approximation, it will then result in the nuclear reactions induced by the atomic deuteron beam with the energy \(E_d = E_{d2}/2\) or \(E_{d3}/3\), \(E_{d2}\) and \(E_{d3}\) being the molecular beam energies in the laboratory system [18]. However, Coulomb explosion of the molecular beam produces an energy spread in the deuteron beam energy [10]. In the case of \(^2\text{D}^+\text{He}\) and \(^3\text{D}^+\text{He}\) beams, the deuteron beam energy is given by

\[
E_d = \frac{E_{d2}}{2} + \frac{e^2}{2r} + \sqrt{\frac{e^2 E_{d2}}{r}} \cos \theta \quad (\text{for } ^2\text{D}^+\text{He}) \tag{7}
\]

\[
E_d = \frac{E_{d3}}{3} + \frac{e^2}{r} + \sqrt{\frac{4e^2 E_{d3}}{3r}} \cos \theta \quad (\text{for } ^3\text{D}^+\text{He}) \tag{8}
\]

in the laboratory system if one assumes that the Coulomb energy of the molecule is converted into the kinetic energy of atoms. Here, \(r\) is the internuclear distance inside the molecule and \(\theta\) is the angle between the incident direction of the molecule and the direction to which one of the deuterons is scattered in the rest frame of the center-of-mass of the molecule after the Coulomb explosion. We have ignored any intrinsic degrees of freedom of the \(^2\text{D}^+\text{He}\) and \(^3\text{D}^+\text{He}\) molecules except for \(r\), which is used to estimate the energy release by the Coulomb explosion. If we denote the true screening energy at \(E = \frac{E_{d2}}{2}\) and at \(E = \frac{E_{d3}}{3}\) for the diatomic \(^2\text{D}^+\text{He}\) and triatomic \(^3\text{D}^+\text{He}\) beams, respectively, by \(U_e^{(t)}\), the energy spreading given by eqs. (7) and (8) will lead to the following apparent screening energy \(U_e^{(a)}\)

\[
U_e^{(a)} = \frac{E}{\pi \eta(E)} \left[ \frac{1}{4\pi} \int_0^\pi 2\pi \sin \theta \exp \left\{ \pi \eta(E) \left( \frac{U_e^{(t)}}{E} + \left( \frac{e^2}{2r} + \sqrt{\frac{e^2 E_{d2}}{r}} \cos \theta \right) \times \frac{1}{2} \right) \right\} d\theta \right] \quad (\text{for } ^2\text{D}^+\text{He}) \tag{9}
\]
TABLE II: The apparent screening energy caused by the Coulomb explosion $U_e^{(a)}$ at each molecular beam energy.

| $E$ (keV) | $U_e^{(a)}$ (eV) | $E$ (keV) | $U_e^{(a)}$ (eV) |
|----------|----------------|----------|----------------|
| 6.02     | 155.2          | 5.01     | 213.0          |
| 6.45     | 154.1          | 5.50     | 209.8          |
| 6.90     | 153.0          | 6.01     | 206.7          |
| 7.51     | 151.8          |          |                |
| 8.18     | 150.5          |          |                |
| 9.02     | 149.2          |          |                |

$U_e^{(a)} = \frac{E}{\pi \eta(E)} \log \left[ \frac{1}{4\pi} \int_{0}^{\pi} 2\pi \sin \theta \exp \left\{ \pi \eta(E) \frac{U_e^{(t)} + \left( \frac{e^2}{r} + \sqrt{\frac{4e^2E_{d3}}{3r}} \cos \theta \right)}{E} \times \frac{1.2}{2} \right\} d\theta \right]$ (for $D_3^+$ beam) (10)

where the factor $1.2/2$ transforms the energy from the laboratory to center-of-mass systems.

TABLE II shows thus estimated apparent screening energy $U_e^{(a)}$ at each molecular beam energy. $E$ is the equivalent atomic deuteron energy in the center-of-mass system at which experiments were carried out [18]. The value $U_e^{(c)} = 117.5$ eV in TABLE II which includes the effect of electron capture by the projectile deuteron, has been used for $U_e^{(t)}$, and $r = 1.17$, 0.97 Å for $D_2^+$, $D_3^+$ molecules, respectively [10]. Interestingly, the apparent screening energy $U_e^{(a)} = 213.0$ eV at the lowest energy $E = 5.01$ keV is about twice as large as the true screening energy and is almost the same as the experimentally reported value $U_e = 219 \pm 7$ eV [18].

The large discrepancy between the true and apparent screening energies can be understood by transforming eq. (10) into

$$U_e^{(a)} = \frac{E}{\pi \eta(E)} \log \left[ \frac{1}{1.2} \int_{U_e^{\min}}^{U_e^{\max}} \sqrt{\frac{3r}{4e^2E_{d3}}} \exp \left( \pi \eta(E) \frac{U_e}{E} \right) dU_e \right]$$ (11)
with

\[
U_{e}^{\text{min, max}} = U_{e}^{(t)} + \left( \frac{e^2}{r} \mp \sqrt{\frac{4e^2E_{d3}}{3r}} \right) \times \frac{1.2}{2},
\]

(12)

where \(\mp\) corresponds to the upper index \(\text{min}\) and \(\text{max}\), respectively. FIG. 1 shows the enhancement factor of the cross section \(f\) as a function of the screening energy, where the relevant region of the energy spread \([U_{e}^{\text{min}}, U_{e}^{\text{max}}]\) is indicated as well as the position of the true screening energy \(U_{e}^{(t)}\) by assuming the case of \(D_{3}^{+}\) beam with \(E = 5.01\) keV. The rapid increase of the enhancement factor within the range of the energy spread \([U_{e}^{\text{min}}, U_{e}^{\text{max}}]\) is the origin of the large apparent screening energy \(U_{e}^{(a)}\).

Our estimate of the energy spread due to the Coulomb explosion is nearly the same as that in [18]. The authors in [18], however, ignored the effects of Coulomb explosion by attributing its justification to [20, 21, 22, 23, 24] which claim that the Coulomb explosion is much gentler and the actual energy spread is much smaller. [21] reports that \(H^{+}-H^{+}\) fragment pair are not observed in the dissociation of 10 keV \(H_{2}^{+}\) ions incident on \(H_{2}\) target. [18] also claims that the good agreement of the data points obtained with the atomic and diatomic beams at nearly overlapping energies confirms that the effects of Coulomb explosion are negligible. [24] studied the collisional dissociation of 20.4 keV \(H_{2}^{+}\) in the \(H_{2}, D_{2}, He, Ne, Ar, Kr\) and \(Xe\) targets, that of 10.2 keV \(H_{2}^{+}\) in the \(Ar\) target and that of 20.4 keV \(D_{2}^{+}\) in the \(Ar\) target and has shown that the collisional dissociation of \(H_{2}^{+}\) is dominated by the process, where it is first excited to the \(2p\sigma_{u}\) state, and then dissociates and that \(D_{2}^{+}\) ions behave in a
similar way as the H$_2^+$ ions concerning the transitions of electrons. 

also pointed out the important role played by the dissociation after the excitation of the vibrational continuum and that by the relative orientation of the molecular axis to the direction of the collision. We have so far ignored these effects. It will be highly desirable to examine both experimentally and theoretically if the same conclusions as those in hold for the Coulomb explosion of D$_2^+$ and D$_3^+$ ions in $^3$He gas target.

V. SUMMARY

We have discussed the effects of electron capture by the projectile ion and the Coulomb explosion in the case of molecular beams. We have first shown that the electron capture increases the screening energy for the D(d,p)T and D($^3$He,p)$^4$He reactions, and that the effective screening energy $U_0^{(c)}$ can get as large as the value observed in experiments. We have then considered the $^3$He(d,p)$^4$He reactions at ultra low energies induced by D$_2^+$ and D$_3^+$ beams, and have shown that the Coulomb explosion can lead to a large apparent screening energy, which is almost twice as large as the adiabatic limit and matches with the value reported by the experimental analysis which ignores the effects of Coulomb explosion. We have assumed the prompt explosion of the molecular ions by the loss of electrons due to exchange process. In view of former studies, however, more detailed studies of the Coulomb explosion will be needed in order to draw a definite conclusion. As we have implicitly postulated, we are especially interested in the Coulomb dissociation caused by the transfer of electrons from the molecular projectiles to the target gas in the same mechanism as that to establish the equilibrium charge and also the neutralization of thus synthesized ions. Whether these processes occur significantly or not when the molecular D$_2^+$ and D$_3^+$ beams propagate through the $^3$He gas target will be discussed in a subsequent paper.
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