

One- and two-electron atomic screening in fusion reactions

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Recent laboratory experiments have measured fusion cross sections at center-of-mass energies low enough that the effects of atomic electrons are important. To extract the cross section for bare nuclei from these data (as required for astrophysical applications), it is necessary to understand these screening effects. We present a model in which the evolution of the electron wave function is treated dynamically in the time-dependent Hartree-Fock scheme, while the motion of the nuclei is treated classically. We have calculated screening in the $d + {}^2\text{H}$ and $d + {}^3\text{He}$ reactions and give the effective screening energy U_e at small internuclear separations as a function of E . The resulting U_e values do not exceed the previously established adiabatic limits, and thus cannot explain the higher screening energies derived from experiment.

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I. INTRODUCTION AND MOTIVATION

At energies below the Coulomb barrier, the cross section for the fusion of two light nuclei drops very rapidly as the center-of-mass energy E is decreased. This drop is due to the exponentially decreasing penetrability of the Coulomb barrier, which for low energies is given by $\exp[-2\pi\eta(E)]$, where $\eta(E) = Z_1 Z_2 \alpha (2E/\mu c^2)^{-\frac{1}{2}}$ is the Sommerfeld parameter for initial nuclei of atomic numbers Z_1, Z_2 and reduced mass μ . Usually, the penetrability and a kinematic factor ($\propto E^{-1}$) are factored out of the cross section by writing

$$\sigma(E) = \frac{S(E)}{E} \exp[-2\pi\eta(E)], \quad (1)$$

where all of the effects of the nuclear physics are embodied in the “ S factor” $S(E)$, which is (barring any sharp resonances) a much more slowly varying function of energy than $\sigma(E)$.

Recent laboratory experiments have measured fusion cross sections for light nuclei down to $E \approx 3$ keV by using both gas and solid targets. At such low energies, the electrons can screen the Coulomb repulsion between the bare nuclei, invalidate the energy dependence expected from (1) with $S(E)$ constant, and significantly raise the measured cross section over that due to the bare nuclei alone [1]. This enhancement of the cross section due to electron screening has been experimentally verified recently for several light nuclear systems [2–4], with the ${}^3\text{He}(d, p){}^4\text{He}$ reaction being the most prominent example [2].

The classical turning radius for a head-on collision is $r_t = Z_1 Z_2 e^2 / E$. Even for the lowest energy cross sections measured, this turning radius is well inside the electron cloud of the target. For example, in the $d + {}^3\text{He}$ collision at $E = 6$ keV, the turning radius is $r_t \approx 0.005$ Å. Thus, in the simplest picture, the effect of electron screening is to provide a constant additional energy U_e to the center-of-mass energy of the colliding nuclei [1]. The enhancement of the cross section is then simply

$$\begin{aligned} f &\equiv \frac{\sigma(E + U_e)}{\sigma(E)} \\ &= \frac{S(E + U_e)}{S(E)} \frac{E}{E + U_e} \frac{\exp[-2\pi\eta(E + U_e)]}{\exp[-2\pi\eta(E)]} \\ &\approx \exp \left\{ \pi\eta(E) \frac{U_e}{E} \right\} \end{aligned} \quad (2)$$

since $U_e \ll E$ and S is essentially energy independent.

The value for the screening energy U_e is known in two limiting cases: when the velocity of the projectile is much larger (sudden limit) or much smaller (adiabatic limit) than the Bohr velocity $v_B = Z\alpha c$. In the sudden limit, the obvious assumption is that the electronic wave function remains constant throughout the collision. The projectile ion then “falls” through the target’s electron cloud before colliding with the nucleus. If we denote the depth of the potential well of the target atom’s electrons by V_e , the projectile (of charge Z_2) gains energy $Z_2 V_e$ in the laboratory system. Of this energy, only the fraction μ/m_2 is available in the center of mass of the colliding particles. Thus, for high projectile velocities, we expect $U_e = 13.6$ eV in the case of $d + {}^2\text{H}$ and $U_e = 54$ eV in the case of $d + {}^3\text{He}$, which are the two systems we are concerned with in this paper. (We use the symbols d , ${}^2\text{H}$, and ${}^3\text{He}$ to denote the bare deuteron, atomic deuterium, and atomic helium, respectively.) In the adiabatic limit, the electrons remain in the lowest energy state of the combined projectile and target “molecular” system that has the same quantum numbers as the original system. For the $d + {}^3\text{He}$ system in this limit, $U_e = 119$ eV, the difference in atomic binding energies between He and Li^+ . For $d + {}^2\text{H}$, $U_e = 20.4$ eV assuming an equally weighted linear combination of the lowest-energy gerade and ungerade wave functions for the electron [5]. If instead only an initial gerade wave function is assumed, one would find that $U_e = 40.7$ eV.

An analysis of electron screening effects on low-energy fusion cross sections is usually performed by applying Eq. (2) to the data and determining a best-fit value for

the screening energy U_e . All such analyses to date have resulted in a value for U_e larger than the adiabatic limit (see [6] for an overview). This discrepancy was confirmed in a recent study that calculated the screening effects of the two electrons in the atomic ${}^3\text{He}$ gas target on the low-energy ${}^3\text{He}(d,p){}^4\text{He}$ data [7]. In this calculation, the nuclear degrees of freedom were described by a microscopic multichannel resonating group model, while the two electrons were treated in the adiabatic approximation, deriving the screening potential from a path integral Monte Carlo calculation. This calculation clearly underestimated the observed screening effects, suggesting the need to consider the coupling of electronic and nuclear degrees of freedom.

In this paper we present a calculation of the electron screening effects in the one-electron $d+{}^2\text{H}$ system and the experimentally well studied two-electron $d+{}^3\text{He}$ system. We describe the coupling of electronic and nuclear degrees of freedom by the time-dependent Hartree-Fock (TDHF) method. That is, we assume that, beyond the classical turning point, the nuclei behave like classical particles, subject to the forces they exert on each other and the force exerted on them by the electrons. However, the electrons are treated quantum mechanically by the TDHF scheme, the wave functions evolving in the time-dependent potential generated by the two nuclei. In this way, we determine the screening potential $U(r)$ between the two nuclei and, by equating $U_e = U(r_t)$, the screening energy. Our dynamical treatment then allows us to check whether the coupling of electron and nuclear degrees of freedom causes the screening energy to exceed the adiabatic limit, as suggested by the experimental data. Unfortunately, we find that the adiabatic limit is not exceeded.

Our paper is organized as follows. In Sec. II, we briefly describe the TDHF method applied in our calculation, as well as the numerical methods involved. Our results are presented and discussed in Sec. III.

II. THE TDHF METHOD

In the case of $d+{}^2\text{H}$, we assume that the target is ground-state atomic deuterium and that the projectile is fully ionized. The wave function describing the electron evolves through the Schrödinger equation

$$i \frac{\partial \psi(\mathbf{r}, t)}{\partial t} = - \left(\Phi(\mathbf{r}, t) + \nabla^2 \right) \psi(\mathbf{r}, t) \quad (3)$$

where

$$\Phi(\mathbf{r}, t) = \frac{1}{|\mathbf{r} - \mathbf{R}_1(t)|} + \frac{1}{|\mathbf{r} - \mathbf{R}_2(t)|} \quad (4)$$

is the potential due to the target and projectile deuterons at locations \mathbf{R}_1 and \mathbf{R}_2 , respectively. In these equations and those following, we have chosen atomic units ($e = \hbar = 2m = 1$).

In the case of $d+{}^3\text{He}$, we assume that the target helium atom is initially in its Hartree-Fock ground state and that the projectile deuteron is ionized. We can then write the

electronic wave function as

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, t) = \psi(\mathbf{r}_1, t) \psi(\mathbf{r}_2, t) \frac{1}{\sqrt{2}} [\alpha(1)\beta(2) - \beta(1)\alpha(2)] . \quad (5)$$

This wave function describes two electrons in a spin-singlet state (α and β are the one-electron spin states), so that the spatial wave function ψ for each obeys Eq. (3) with

$$\Phi(\mathbf{r}, t) = \frac{Z_1}{|\mathbf{r} - \mathbf{R}_1(t)|} + \frac{Z_2}{|\mathbf{r} - \mathbf{R}_2(t)|} - \int d^3\mathbf{r}' \frac{|\psi(\mathbf{r}', t)|^2}{|\mathbf{r} - \mathbf{r}'|} \quad (6)$$

where \mathbf{R}_1 is the position of the target ${}^3\text{He}$ nucleus, \mathbf{R}_2 is the position of the projectile deuteron, and the integral is the potential due to the other electron.

In accordance with our classical treatment of the nuclei, the time dependence of the nuclear position vectors $\mathbf{R}_i(t)$ is determined from Newton's law, where the force on each nucleus is the sum of the Coulomb force of the other nucleus and the force due to the electronic charge density.

Since impact parameters that lead to nuclear reactions are small on the atomic scale, we can assume a vanishing impact parameter when simulating the collision's effect on the electron(s). This assumption, when combined with the initial spherical symmetry of the target wave function, means that the wave function is azimuthally symmetric about the collision axis. It is then convenient to express the wave function in cylindrical coordinates as $\psi(\rho, z, t)$ and to use the evolution method of [8]. For the $d+{}^2\text{H}$ calculations, we used $\Delta\rho = \Delta z = 0.1$ atomic unit, with $N_\rho = 50$ grid points along the ρ axis and $N_z = 249$ grid points along the z axis. The smaller spatial extent of the atomic wave function in the $d+{}^3\text{He}$ calculation allowed us to use $\Delta\rho = \Delta z = 0.06$ atomic unit.

The initial state of the target atom was prepared by evolving a trial wave function in imaginary time [9]. The resulting HF ground state is the lowest eigenfunction of the discretized Hamiltonian. As long as the overlap between the ground state and the trial wave function is nonzero, this method will converge to the ground state. The converged energy of the ${}^2\text{H}$ ground state was -0.504 Hartree, and the converged energy of the He ground state was -2.824 Hartree. These values can be compared with the experimental values of -0.50 Hartree and -2.901 Hartree, respectively, and the exact HF value of -2.861 Hartree.

III. RESULTS AND DISCUSSION

Figures 1 and 2 show the time evolution of the electron wave function in the $d+{}^2\text{H}$ and $d+{}^3\text{He}$ systems, represented in the usual way by contour plots of the electron density, $|\Psi(\mathbf{r}, t)|^2$ and $2|\Psi(\mathbf{r}, t)|^2$, respectively. The contours cover the density above 2×10^{-4} in equal steps on a logarithmic scale. In both cases, the energies of the colliding nuclei have been chosen between the sudden and adiabatic limits: $E = 25$ keV for the $d+{}^2\text{H}$ system and

$E = 20$ keV for the $d+^3\text{He}$ system.

For both the $d+^2\text{H}$ and $d+^3\text{He}$ systems, the electron densities show significant asymmetries when the two nuclei approach each other. This signals the presence of configurations other than s waves in the electron wave function and in the case of $d+^3\text{He}$ clearly indicates that the system has not yet reached the adiabatic limit at this energy. In the $d+^2\text{H}$ system there should be a p wave present even in the adiabatic limit [5]. If we repeat the TDHF calculations at $E = 5$ keV and project the final states onto the eigenstates of the Hamiltonian, the wave functions show the behavior expected in the adiabatic limit.

During the collision, the force along the internucleon separation on each nucleus due to the electron(s) is given by

$$F_i(t) = Z_i \int d^3\mathbf{r}' \frac{\rho(\mathbf{r}', t)[(\mathbf{R}_i(t) - \mathbf{r}') \cdot \hat{\mathbf{z}}]}{|\mathbf{R}_i(t) - \mathbf{r}'|^3}. \quad (7)$$

Thus, the relative force exerted by the electrons is $F_{\text{rel}} = F_1 - F_2$. As a typical example, Fig. 3 shows the relative force exerted by the two electrons on the colliding $d+^3\text{He}$ nuclei at $E = 20$ keV, corresponding to the situation of Fig. 2. The electrons induce an attractive force on the

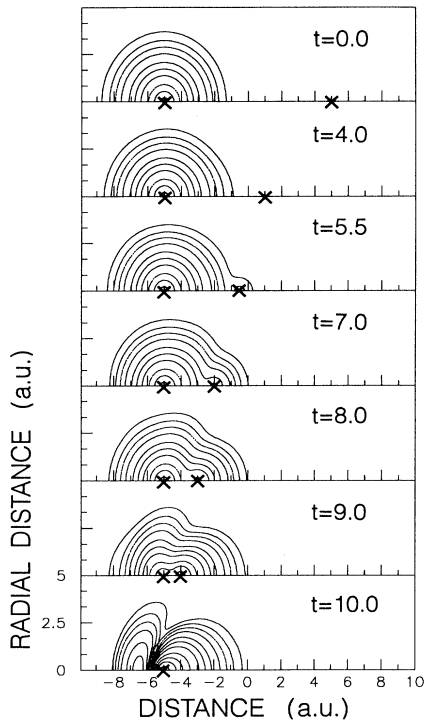


FIG. 1. Evolution of the electron wave function in the $d+^2\text{He}$ system at a collision energy $E = 25$ keV. The plot shows contours of the electron density, equally spaced on a logarithmic scale; neighboring lines indicate a change in density by a factor $10^{1/3}$. The positions of the two nuclei are indicated by crosses. The first plot corresponds to the starting configuration, while the last shows the electron density at the internuclear separation $r_t = 58$ fm, the classical turning point.

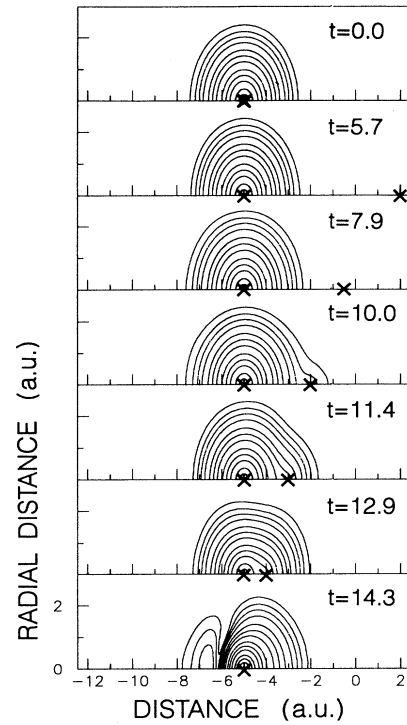


FIG. 2. Similar to Fig. 1, but for the $d+^3\text{He}$ system at $E = 20$ keV.

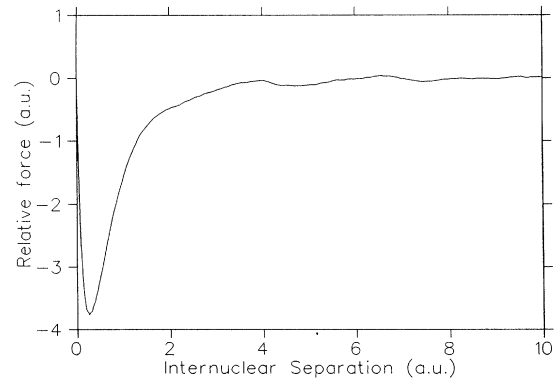


FIG. 3. The relative force \mathbf{F}_{rel} exerted by the two electrons on the colliding $d+^3\text{He}$ nuclei at $E = 20$ keV.

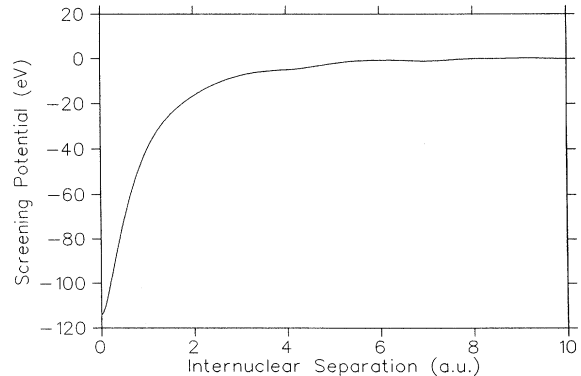


FIG. 4. The electron screening potential $U(r)$, corresponding to the collision shown in Figs. 2 and 3.

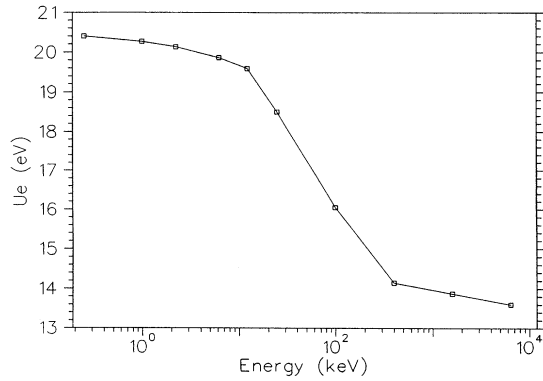


FIG. 5. The screening energy U_e as a function of energy for the $d+^2\text{H}$ system. The values corresponding to the adiabatic and sudden limits are marked at the left and right scales, respectively.

nuclei, thus accelerating their approach. This force is strongest at separations of order 0.2 \AA and, as expected, decreases linearly at smaller distances. The “bumps” on the tail of the curve are an indication of charge-exchange processes; they are even more pronounced in the $d+^2\text{H}$ case, where the projectile and target nuclei have equal charges.

From F_{rel} , the electron-induced screening potential $U(r)$ is obtained by integration. The potential corresponding to the $d+^3\text{He}$ collision of Fig. 3 is shown in Fig. 4. At small internuclear separations, $r \lesssim r_t = 0.005 \text{ \AA}$, $U(r)$ becomes constant reflecting the fact that the two nuclei are well inside the electron cloud and the electrons effectively feel only the charge of the combined system. For the collision depicted in Fig. 3, we find $U(r_t) = 114 \text{ eV}$, which is slightly smaller than the adiabatic limit, $U_e = 119 \text{ eV}$.

If we define the screening energy U_e to be the screening potential at the classical turning point and plot this as a function of E , we arrive at Fig. 5 and Fig. 6 for the $d+^2\text{H}$ and $d+^3\text{He}$ systems, respectively. In either case, our calculated screening energies recover the values for the sudden and adiabatic limits at large and small collision energies, respectively. Further, for the $d+^3\text{He}$ case, the adiabatic limit is reached approximately at energies $E \leq 20 \text{ keV}$, in accord with the assumptions of Ref. [1]. At higher energies, this limit is obviously not valid. However, here the ratio $U_e/E^{3/2}$ appearing in the exponential in Eq. (2) (and thus determining the energy dependence of the enhancement factor f) becomes very small, so that electron screening effects can be ignored altogether.

Our calculations show a continuous transition from the

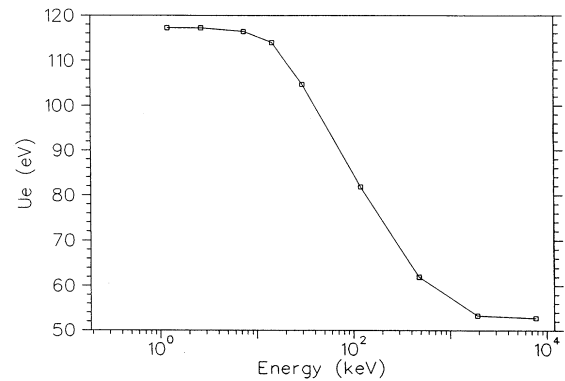


FIG. 6. Similar to Fig. 5, but for the two-electron $d+^3\text{He}$ system.

adiabatic to the sudden limit as the collision energy increases. Importantly, the calculated screening energy never exceeds the adiabatic limit. Thus, our dynamical TDHF calculation cannot explain why experiments evidently observe larger electron screening effects than obtained in the adiabatic approach. If this behavior is in fact real, then it obviously challenges our understanding of low-energy nuclear collisions in the presence of atomic electrons. As our calculation clearly indicates that the experimental screening effects cannot be reproduced by treating the electrons on the mean field level, a reasonable next step is to describe, also, the nuclei quantum mechanically, in this way accounting for the momentum distribution of the electrons and the related recoil effects on the colliding nuclei. Work in this direction is in progress.

Because of its astrophysical importance, it is critically important that the discrepancy between theoretical predictions and the experimental observations of laboratory electron screening effects be resolved, in order to make effective use of the remarkable efforts currently being made to push laboratory cross section measurements to ever lower energies. This calls both for improved theoretical studies of these effects and for their independent experimental verification.

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