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# Scattering and $(e,2e)$ reactions in classical $s$-wave helium

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We study the classical collisions of electrons with one-electron atoms or ions in a model where both electrons are restricted to spherical states. At negative total energy, we calculate the probability for bound motion of both electrons occurring—as opposed to undelayed direct or exchange scattering. At positive total energy, we calculate the probability for $(e,2e)$ reactions. There is a finite threshold for the onset of $(e,2e)$ reactions. Its value depends on the nuclear charge and can be deduced from a simple transcendental equation. The general behavior of the probability for $(e,2e)$ reactions as a function of energy is quite similar to the results of quantum-mechanical calculations and to experimental data.

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## I. INTRODUCTION

The correlated motion of two electrons in an atom is still largely an unsolved problem, even though there has been considerable experimental [1,2] and theoretical [3–9] progress in recent years. One of the simplest models for two electrons interacting with each other and with a nucleus via long-range Coulomb forces is $s$-wave helium, where both electrons are restricted to spherical states with individual angular momentum equal to zero. Classically $s$-wave helium corresponds to two spherical shells of charge $-1$ expanding and contracting around a fixed nucleus of charge $Z$.

In a recent paper [10] we presented a comprehensive account of the bound motion of classical $s$-wave helium at negative total energy. Important results were the following: periodic orbits are unstable; nonperiodic trajectories can unambiguously be assigned an ionization time or a scattering time delay; ionization times impose a fractal structure on phase space; the initial conditions of nonionizing trajectories form a Cantor set; almost all bound trajectories ionize, but the mean lifetime with respect to autoionization, averaged over all initial conditions, is infinite. Fractal structures have also been observed in recent investigations of classical helium in three dimensions [7,9]. The similarity of many results obtained in [9] and [10] gives hope that much of the physics of the simpler and more transparent $s$-wave model is also relevant for the realistic three-dimensional case.

The present study of $s$-wave helium deals mainly with the case of unbound motion, where at least one of the electrons has positive energy. If we start with incoming boundary conditions of one electron, then the outgoing trajectory may correspond to one bound electron with negative energy and one free electron with positive energy, or to two free electrons. The former case corresponds to direct or exchange scattering, and can occur at negative, vanishing, or positive total energy. The latter case corresponds to an $(e,2e)$ reaction and can only occur at positive total energy. At negative total energy we calculate, as a function of the energy of the incoming electron, the probability for the occurrence of bound motion as opposed to undelayed direct or exchange scattering. At positive energy we calculate the probability for $(e,2e)$ reactions. A precise study of the possible trajectories reveals that, contrary to naive expectation, there is a finite positive threshold for the onset of $(e,2e)$ reactions, which is proportional to the binding energy of the initially bound electron and depends on the nuclear charge $Z$.

## II. MODEL

The Hamiltonian function of classical $s$-wave helium is, in atomic units,

$$H(r_1,r_2)=\frac{p_1^2}{2}-\frac{Z}{r_1}+\frac{p_2^2}{2}-\frac{Z}{r_2}+\frac{1}{r_>}$$
$$=\frac{p_1^2}{2}+\frac{p_2^2}{2}-\frac{Z}{r_<}-\frac{Z-1}{r_>}\,, \tag{1}$$

where $r_<$ is the smaller and $r_>$ the larger of the radial coordinates $r_1,r_2$ of the two electrons. Within the regions $r_1>r_2$ (region 1) and $r_1<r_2$ (region 2), the equations of motion generated by (1) are separable and describe one-dimensional Kepler motion in each of the two uncoupled coordinates:

$$\frac{p_1^2}{2}-\frac{Z-1}{r_1}=E_1\,,\quad \frac{p_2^2}{2}-\frac{Z}{r_2}=E_2\quad \text{(region 1)}\,, \tag{2}$$

$$\frac{p_1^2}{2}-\frac{Z}{r_1}=E_1\,,\quad \frac{p_2^2}{2}-\frac{Z-1}{r_2}=E_2\quad \text{(region 2)}\,. \tag{3}$$

Within each region the energies $E_1$ and $E_2$ for the two degrees of freedom are conserved, but the only global constant of motion is the total energy $E=E_1+E_2$. Coupling between the two degrees of freedom occurs on the line $r_1=r_2$ in the $r_1,r_2$ plane, where the potential has a kink. When a trajectory crosses this line there is a sudden change of acceleration but no discontinuity in velocities. If such a crossing occurs at $r_1=r_2=s$, then the energy $1/s$ is transferred from the initially outer electron to the other electron, i.e., after an encounter of the two electrons at $r_1=r_2=s$ the now outer electron has gained the energy $1/s$ at the expense of the now inner electron [10].

Since the potential in (1) is homogeneous, the equations of motion can be scaled to energy-independent form. It is only necessary to distinguish between negative, vanishing, or positive total energy. Each trajectory can be identified by two parameters, such as an initial position on the $r_1$ axis ($r_2=0$) and the corresponding initial momentum $p_1$ in the $r_1$ direction. Alternately, we might choose the initial partitioning $E_1/E_2$ or $|E_1/E_2|$ of the energies of the two electrons as one of the two independent parameters needed to specify a trajectory.

## III. RESULTS

### A. Negative total energy

When there is bound motion of the two electrons (i.e., both $E_1$ and $E_2$ are negative) then such bound motion exists between an initial and a final encounter of the electrons on the line $r_1=r_2$. Before the initial and after the final encounter one electron always has positive energy and there are no further encounters of the two electrons. The scattering time delay can be defined unambiguously as the duration of bound motion, i.e., the time between two encounters initiating and terminating the bound motion [10].

If we start with incoming boundary conditions of one electron (electron 1, say, $E_1>0$), then the first encounter with the initially bound electron 2 ($E_2<0$) at $r_1=r_2=s$ need not lead to bound motion of both electrons, even if the total energy is negative.

If the energy transfer $1/s$ is less than $E_1$, then electron 1, which becomes the inner electron, retains positive energy at the encounter and then acquires a larger energy at the subsequent encounter, at which it again becomes the outer electron. The subsequent encounter is inevitable, because electron 2 is still bound and electron 1 moves outwards (with positive energy) after reflection at $r_1=0$. This simple mechanism for direct scattering after two encounters can only occur if the amplitude of oscillation of the initially bound electron, which is $Z/|E_2|$ according to (2), is greater than $1/E_1$, i.e., for $E_1/|E_2|>1/Z$.

If the energy transfer $1/s$ at the first encounter is larger than $|E_2|$, then electron 2, which becomes the outer electron, acquires positive energy. This leads to immediate exchange scattering if there are no further encounters, or to direct scattering if there is a second encounter. It can be shown [11] that, if the first encounter of the two electrons does not lead to bound motion (i.e., negative energies of both electrons), then no further encounters lead to bound motion. Scattering processes in which the first encounter does not lead to bound motion of both electrons correspond to exchange scattering after just one encounter of the two electrons or to direct scattering after two encounters. In both cases the scattering time delay is zero if we define it as the duration of simultaneous bound motion of the two electrons.

Trajectories leading to bound motion or to undelayed scattering are illustrated in Fig. 1 for the case of negative

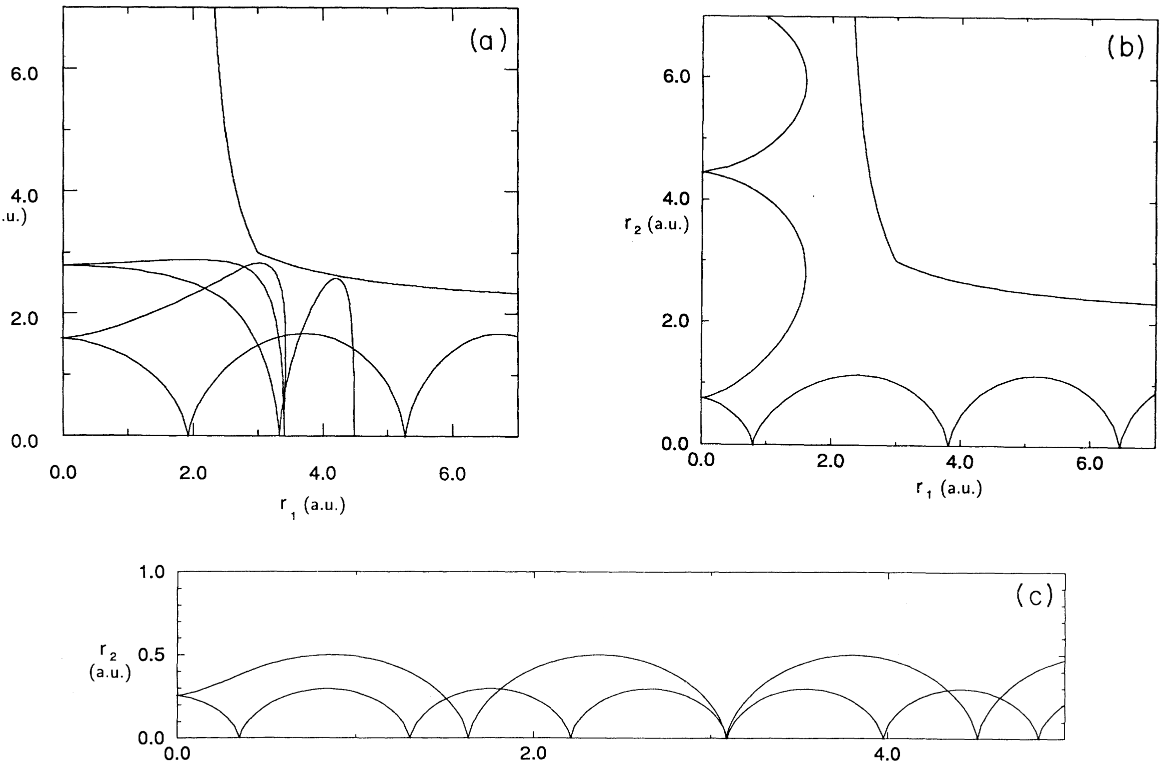

FIG. 1. Trajectories leading to bound motion (a), undelayed exchange scattering (b), and undelayed direct scattering (c) for the case of negative total energy. Here $Z=2$ and $r_1,r_2$ are in atomic units. In (a) and (b) the equipotential line $-Z/r_< -(Z-1)/r_> = -1$ is also shown.

total energy corresponding to $E_1 < |E_2|$, $1/|E_2| < 1/E_1$. Figure 1(a) shows initial conditions leading to bound motion after an initial encounter in the range $1/|E_2| < s < 1/E_1$; Fig. 1(b) shows an example of exchange scattering for an initial encounter at $s < 1/|E_2|$; and Fig. 1(c) shows direct scattering for $s > 1/E_1$.

Bound motion occurs for all trajectories whose first encounter at $r_1 = r_2 = s$ is within the range

$$\frac{1}{|E_2|} < s < \frac{1}{E_1} \ . \tag{4}$$

The probability for bound motion can be obtained by counting the number of trajectories which, for given initial energy ratio $E_1/|E_2|$, cross the axis for the first time in the range defined by (4), and comparing with all trajectories of the same initial energy ratio. The unperturbed oscillations of the initially bound electron 2 may serve as a clock to measure the time at which the incoming electron 1 passes a given distance from the nucleus (larger than $Z/|E_2|$ to ensure that it passes prior to the first encounter), and we might choose this starting time as the second parameter defining the trajectories. Such starting times of the incoming electron define the asymptotic phase of the incoming oscillatory trajectory. An alternate second parameter is the position of a collision with the $r_1$ axis where $r_2 = 0$. Because the velocity of the electron is larger closer to the nucleus, the separations between collision points with the $r_1$ axis are stretched by a factor $p_1$ to smaller $r_1$ for trajectories with uniformly spaced starting times. We assume a uniform distribution of trajectories with respect to starting times.

Figure 2 shows (for $Z = 2$) the resulting probability for bound motion as a function of the energy ratio $E_1/|E_2|$ of the incoming electron energy to the binding energy of the initially bound electron. The kink at $E_1/|E_2| = 1/Z = 0.5$ corresponds to the onset of undelayed direct scattering for $s > 1/E_1$, as in Fig. 1(c).

### B. Positive total energy

For positive total energy we have $E_1 > |E_2|$ and direct and exchange scattering are possible, as are $(e,2e)$ reactions in which both electrons leave the nucleus with positive energy. Which reaction follows from given initial conditions again largely depends on the position $s$ of the first encounter of the incoming electron 1 with the initially bound electron 2.

If $s > 1/|E_2|$, then electron 2 remains bound after the first encounter, and after electron 1 is reflected at $r_1 = 0$ there is a second encounter at which the already positive energy of electron 1 gains a further increment, while electron 2 remains bound: we have direct scattering after two encounters. If $s = 1/|E_2|$, then the outer electron 2 has exactly vanishing energy and a second encounter leading to bound motion of electron 2 is also inevitable.

If $s < 1/E_1$, then electron 1 loses the energy $1/s > E_1$ and becomes bound at the first encounter; electron 2, which is now the outer electron, moves away with positive energy, which corresponds to exchange scattering, if there is no further encounter. If a second encounter does occur, it invariably leads to direct scattering and not to an $(e,2e)$ reaction [11].

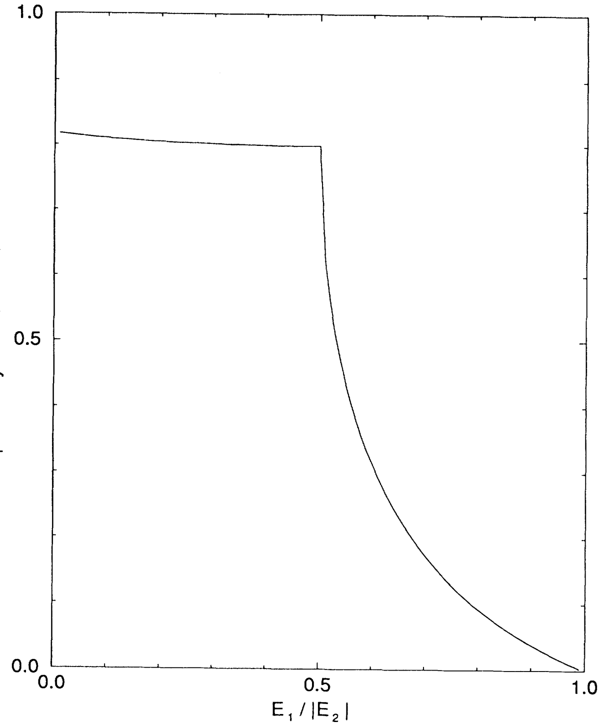

FIG. 2. Probability of bound motion of both electrons occurring for $Z = 2$ as function of the ratio $E_1/|E_2|$ of the energy of the incoming electron to the binding energy of the initially bound electron.

A necessary condition for the occurrence of $(e,2e)$ reactions is thus that the position $s$ of the first encounter of the two electrons lie in the range (see Fig. 3)

$$\frac{1}{E_1} \le s < \frac{1}{|E_2|} \ . \tag{5}$$

However, not all trajectories satisfying (5) lead to an $(e,2e)$ reaction. If, after the first encounter, the outer electron (electron 2) is moving inwards or if it is moving outwards too slowly, then a second encounter can lead to bound motion of electron 2 and hence to scattering. The most favorable conditions for electron 2 escaping are when it acquires the maximum energy allowed by (5) [11]. This occurs if $s = 1/E_1$ and then, after the first encounter, we have

$$E_1^a = 0 \ , \quad E_2^a = E \ , \quad r_1 < r_2 \ . \tag{6}$$

The corresponding trajectory is illustrated for a fixed initial energy $E_1$ of the incoming electron and different total energies $E$ in Fig. 3. After the initial encounter at $s = 1/E_1$ the trajectory is reflected at the $r_2$ axis, and then both electrons move outward. The velocities are given by

$$\begin{aligned} \frac{dr_1}{dt} &= \pm\left[\frac{2Z}{r_1}\right]^{1/2} , \\ \frac{dr_2}{dt} &= \pm\left[2\left[\frac{Z-1}{r_2} + E\right]\right]^{1/2} , \end{aligned} \tag{7}$$

where plus signs describe outward and minus signs inward motion of the respective electrons. An equation for the path in the $r_1, r_2$ plane can be obtained by dividing the two equations (7):

$$\frac{dr_2}{dr_1} = \pm \left[ \frac{r_1}{r_2} \frac{Er_2 + Z - 1}{Z} \right]^{1/2} . \tag{8}$$

The motion between the first encounter at $r_1 = r_2 = s$ and the reflection at the $r_2$ axis is described by (8) with a minus sign in front of the square root, and there is a plus sign for the subsequent motion when both electrons are moving outwards.

After reflection at $r_1 = 0$, the inner electron 1 is initially faster than the outer electron 2, i.e., $dr_2/dr_1 < 1$, as is obvious from Eq. (8), and there may be a second encounter of the two electrons. If this encounter occurs closer than $r_1 = r_2 = 1/E$ to the nucleus, then the energy transfer is so big that electron 2 becomes bound and we have direct scattering. As we show below, this is inevitable for sufficiently small $E$, and hence the onset of $(e,2e)$ reactions does not occur exactly at $E = 0$.

At given energy the most favorable conditions for an $(e,2e)$ reaction are given by (6). If there is, even under

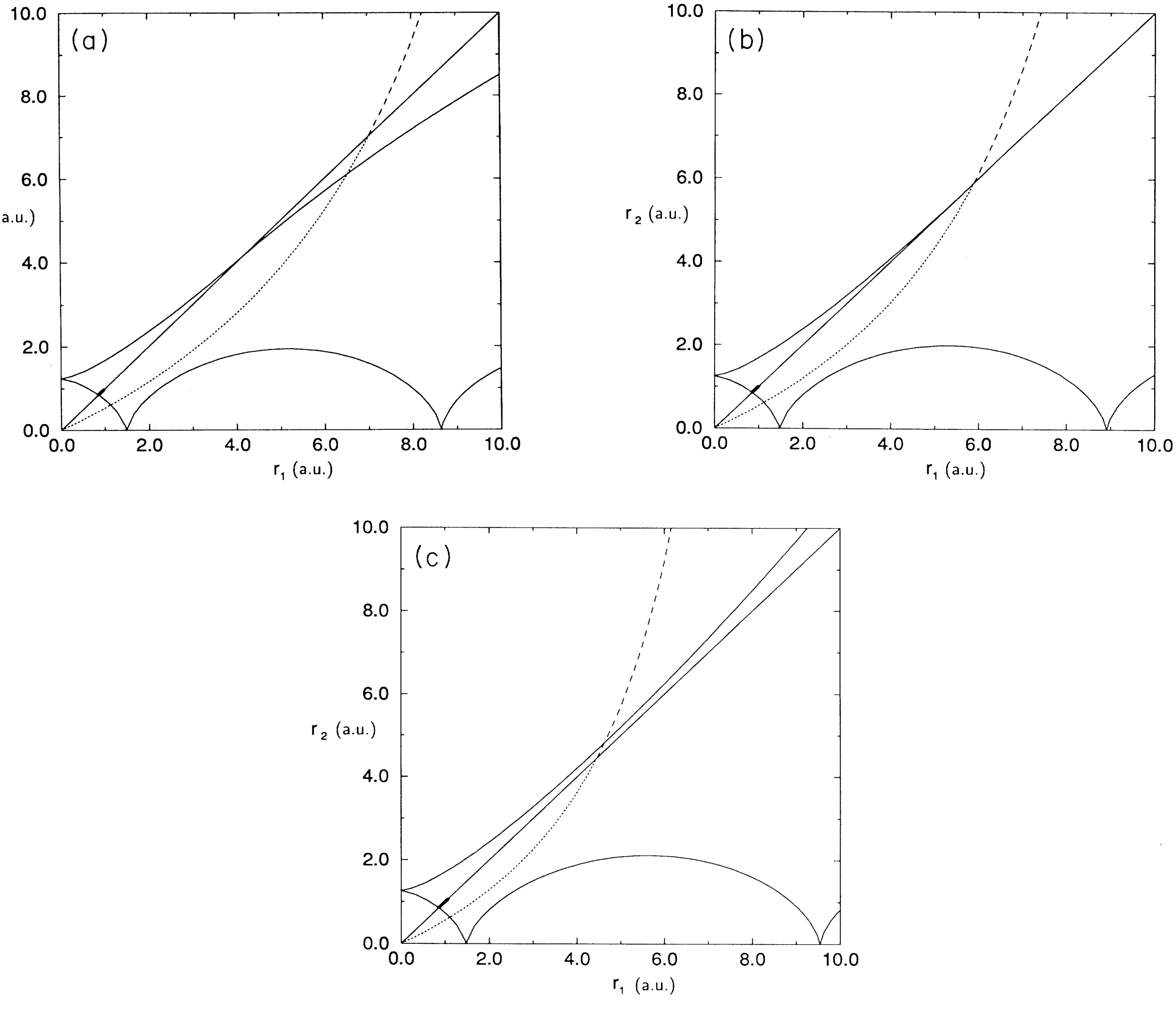

FIG. 3 Trajectory corresponding to the "most favorable conditions" for an $(e,2e)$ reaction according to Eq. (6) (for $Z = 2$). The initial energy of the incoming electron is $E_1 = 1.17$ in all cases. The short fat line shows that part of the diagonal, defined by Eq. (5), where a first encounter of the two electrons must necessarily occur in order to avoid scattering. (a) corresponds to $E_2 = -1.03$ so that the total energy is below the threshold ($\approx 0.17$) for the onset of $(e,2e)$ reactions. Electron 1 is captured after a second encounter at $s < 1/E$. The same happens for other trajectories not corresponding to the most favorable conditions, i.e., for an initial encounter at $s > 1/E_1$. In (b) $E_2 = -1$, so the total energy corresponds to the threshold for $(e,2e)$ reactions. The critical trajectory continues after the first encounter at $s = 1/E_1$ and reflection at the $r_1$ axis to touch the diagonal with unit gradient at $s = 1/E$. At energies above the threshold (c) the "most favorable" conditions define a trajectory along which electron 1 never catches up with electron 2 after the first encounter and both electrons escape. The dashed line is the locus of points defined by (9) where both electrons have the same velocity (in region 2). (The dotted line is its formal extension into region 1.)

these conditions, a further encounter closer than $r_1 = r_2 = 1/E$ and therefore direct scattering, then no $(e,2e)$ reaction is possible at all. Such an encounter can only occur if the outer electron 2 is not faster than the inner electron 1 ($dr_2/dr_1 \leq 1$). The locus of points where $dr_2/dr_1$ is unity corresponding to equal velocities of both electrons follows from (8):

$$r_2 = \frac{(Z-1)r_1}{Z - Er_1} . \tag{9}$$

[Note that (9) is derived from Eq. (7), which are valid only in region 2, $r_1 < r_2$.] If the trajectory reaches the line (9) before reaching the diagonal $r_1 = r_2$, then the outer electron 2 is now faster than electron 1 and it remains faster since the negative acceleration is smaller for the outer electron. Thereby a further encounter is impossible and the trajectory describes an $(e,2e)$ reaction. The minimal energy for $(e,2e)$ reactions is given by a *critical trajectory* which just reaches the diagonal with equal velocities of both electrons ($dr_2/dr_1 = 1$). This takes place at $r_1 = r_2 = 1/E$, which can be seen from (9) [see Fig. 3(b)]. If the total energy is smaller than the energy of this critical trajectory, the outer electron is slower and is overtaken by the inner electron at a point $r_1 = r_2 < 1/E$, which leads to direct scattering.

Thus the minimal energy needed for $(e,2e)$ reactions to be possible is defined by the existence of a critical trajectory which starts at $r_1 = r_2 = 1/E_1$ ($E_1$ being the initial energy of the incoming electron) and touches the diagonal with unit gradient at $r_1 = r_2 = 1/E$, $E$ being the total energy. This critical value of $E$ can be deduced by elementary integration of Eq. (8), which leads to a transcendental equation for the ratio

$$x = \frac{E}{E + |E_2|} , \quad \frac{E}{|E_2|} = \frac{x}{1-x} , \tag{10}$$

namely,

$$Z - \sqrt{Zx(Z-1+x)} + (Z-1)\sqrt{Z} \ln \left[ \frac{\sqrt{Z-1+x} + \sqrt{x}}{\sqrt{Z} + 1} \right] - \tfrac{2}{3}(1 + x^{3/2}) = 0 . \tag{11}$$

Equation (11) defines finite thresholds for the onset of $(e,2e)$ reactions for any charge $Z \geq 1$ of the nucleus. The ratio of the threshold energy to the binding energy of the initially bound electron, $E/|E_2|$, is $\frac{1}{3}$ for $Z = 1$, roughly 0.169 777 for $Z = 2$, and decreases monotonically with $Z$, reaching 0.010 11 for $Z = 100$ (see Fig. 4).

For a given energy $E_1$ above the threshold defined by (11), all trajectories whose first encounter on the line $r_1 = r_2 = s$ is just beyond $s = 1/E_1$ lead to an $(e,2e)$ reaction with no further encounters. Larger values of $s$ correspond to less energy transfer to the outer electron 2, and there may be a second encounter. Before $s$ reaches the upper limit $1/|E_2|$ given by Eq. (5) a situation is reached, where the outer electron 2 is too slow to avoid capture at the second encounter. The stretch of values of $s$ between $1/E_1$ and this upper limiting value leads to $(e,2e)$ reactions, and the probability for $(e,2e)$ reactions can be calculated by comparing with all possible trajectories. As in the calculation of the probability of bound motion above (Fig. 2), we assume that the trajectories are uniformly distributed with respect to starting times of the incoming electron relative to the oscillation of the initially bound electron.

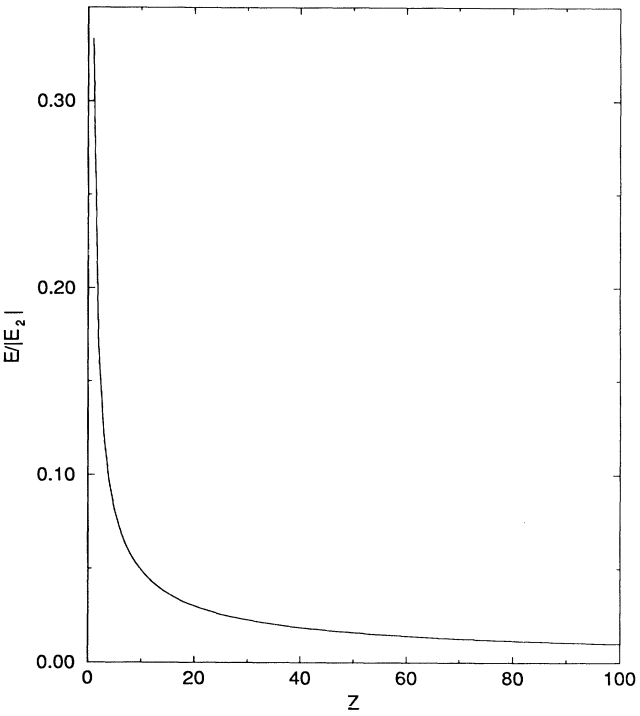

FIG. 4. Finite threshold for the onset of $(e,2e)$ reactions according to Eq. (11). The ratio of total energy to binding energy of the initially bound electron is plotted as a function of the nuclear charge $Z$.

Figure 5 shows resulting probabilities for $(e,2e)$ reactions as functions of the ratio $E_1/|E_2|$ of the initial energy of the incoming electron to the binding energy of the initially bound electron for various values of $Z$. The position of the maximum is at $E_1/|E_2| \approx 4$ and is virtually independent of $Z$. The probabilities do not increase proportional to $1/Z^4$ in accordance with the frequently discussed scaling law for $(e,2e)$ cross sections [12]; in the present case the decrease with $Z$ is closer to a $1/Z$ behavior, especially for high energies.

A comparison of our purely classical calculation with a quantum-mechanical calculation by Callaway and Oza [13] is shown in Fig. 6 for $Z = 1$. Callaway and Oza obtained the elastic and first two inelastic scattering cross sections in a quantum-mechanical calculation restricted to $s$-waves and singlet states. Higher inelastic cross sections were extrapolated on the basis of the Born approximation and the total reaction cross section was deduced from the elastic transition amplitude via the optical theorem. The fraction assigned to $(e,2e)$ reactions was obtained by subtracting the elastic and inelastic scattering contributions from the total cross section. Figure 6 shows the ratio of the resulting $(e,2e)$ cross section to the total cross section together with the probability for $(e,2e)$

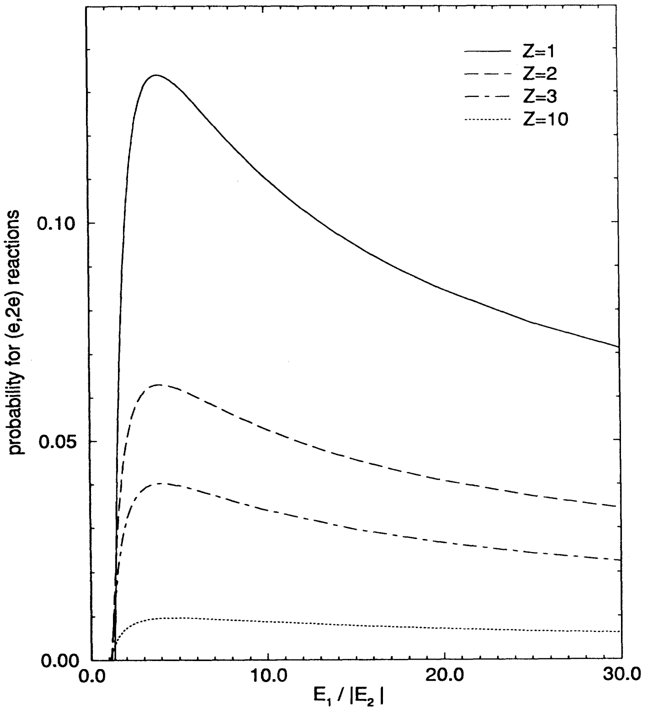

FIG. 5. Probabilities for $(e,2e)$ reactions as functions of the ratio of the initial energy of the incoming electron to the binding energy of the initially bound electron for various values of the nuclear charge $Z$.

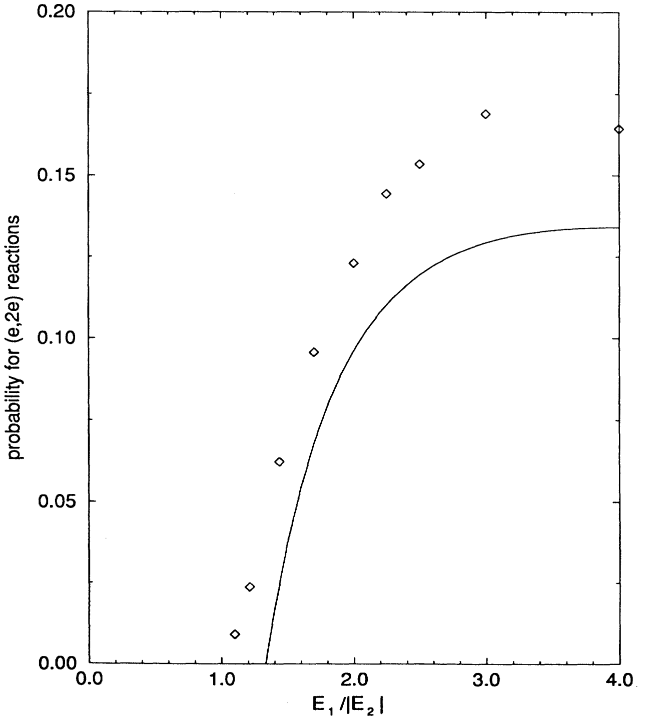

FIG. 6. Probabilities for $(e,2e)$ reactions on neutral hydrogen $(Z=1)$. The solid line shows our classical $s$-wave calculation; the diamonds are the results of a quantum-mechanical calculation [13] in which the contribution due to $(e,2e)$ reactions is obtained by subtracting calculated elastic and inelastic scattering cross sections from a total reaction cross section derived from the elastic transition amplitude via the optical theorem.

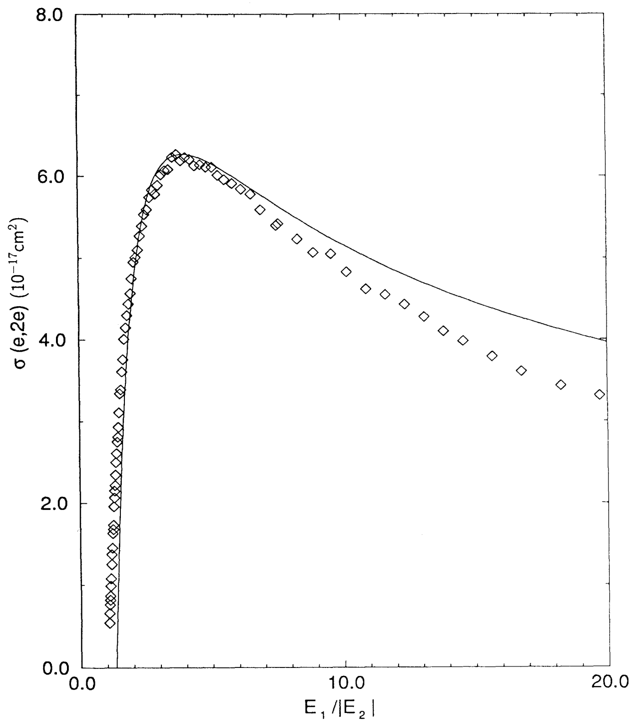

FIG. 7. Probabilities and cross sections for $(e,2e)$ reactions on hydrogen $(Z=1)$. The diamonds are experimental cross sections from [12] in $10^{-17}$ cm$^2$. The solid curve is the result of our classical $s$-wave calculation. The curve was rescaled to have the same height at maximum as the experimental data.

reactions in the classical calculation. Agreement is quite good considering the different underlying theories and inevitable uncertainties in the quantum calculation.

Finally, Fig. 7 shows, again for $Z=1$, the probability for $(e,2e)$ reactions in the classical $s$-wave calculation in comparison with experimental results for $(e,2e)$ cross sections on real hydrogen. The calculated curve has been scaled so that the height of the maximum agrees with the experimental value. The general shapes of the classical $s$-wave probability and the real physical cross section are quite similar, the main difference being in the slower falloff of the classical $s$-wave probabilities at higher energies. One way of translating the dimensionless probability into a cross section would be to multiply by an area, such as the inverse square of the wave number. Such an area would correspond to the range of impact parameters one might assign to zero angular momentum of the incoming electron. In Fig. 7 this multiplication would correspond to dividing the solid line by the incoming energy $E_1$. The resulting curve would then fall off faster than the experimental data towards higher energies.

## IV. SUMMARY

Within the model of classical $s$-wave helium we have calculated the probabilities for bound motion occurring at negative total energy and the probabilities for $(e,2e)$ reactions at positive total energy. The onset of $(e,2e)$ reactions is not at total energy zero, as might be naively expected, but at a finite threshold. This can be understood by realizing that, when both electrons have very small positive energies, the inner electron is always faster and overtakes the other electron, which then becomes bound. The finite threshold is proportional to the binding energy of the initially bound electron and has a monotonically decreasing dependence on the nuclear charge $Z$. Precise values of the threshold can be deduced from the transcendental equation (11).

The general behavior of the probability for $(e,2e)$ reactions calculated as a function of the energy of the incoming electron in the classical $s$-wave model agrees qualitatively with comparable quantum-mechanical calculations and with experimental data.

## ACKNOWLEDGMENT

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