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Ionization of hydrogen by positron impact near the fragmentation threshold

Jan M. Rost and Eric J. Heller
Lyman Laboratories of Physics, Harvard University, Cambridge, Massachusetts 02138
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The semiclassical approximation of Feynman's path integral is used to calculate the S matrix for the positron-impact ionization of hydrogen. The formulation provides a full scattering amplitude, and more importantly does not require knowledge of the asymptotic three-body Coulomb state in the continuum. In the limit of vanishing excess energy, the results confirm Wannier's classical model for fragmentation [Phys. Rev. **90**, 817 (1953)]. The experimentally observable ratio of fragmentation versus total ionization (including positronium formation) is predicted.

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The ionization of hydrogen by positron impact is one of the most fundamental three-body scattering processes which can be experimentally observed [1]. It differs from the ionization by electron impact in two ways: (i) Since all three particles are distinguishable, quantum-mechanical exchange effects are absent. (ii) Besides fragmentation, positronium formation (PF) contributes an additional channel to the ionization of the hydrogen atom. Formally, this is an exchange process (not in the sense of the Pauli principle) where the positron becomes bound to the electron in exchange for the proton. In electron-hydrogen scattering, the corresponding event cannot be distinguished from an excitation of the target electron.

Anticipated measurements in the threshold region [2] motivate this study as well as a fundamental theoretical interest in fragmentation phenomena near threshold. Some theoretical predictions exist in the literature: based on Wannier's classical approach for the threshold ionization of hydrogen [3], Klar predicted in 1982 a power law for the fragmentation cross section near threshold [4]. Temkin concluded from the "dipole theory" that the cross section for ionization should be constant close to $E = 0$ [5]. However, he already mentioned that his approach does not distinguish between the positronium formation channel and fragmentation. Finally, Geltman predicted from a Coulomb distorted-wave (CDW) theory that the fragmentation cross section should be exponentially small at $E = 0$ [6].

We describe the inelastic scattering with a semiclassical S matrix which can be constructed from an approximate evaluation of Feynman's path integral with classical paths. In its semiclassical limit, as given by van Vleck [12] and improved by Maslov and Fedoriuk [13] and Gutzwiller [14], the quantum propagator $\exp[-iHt/\hbar]$ contains only information which can be obtained from the classical paths. Nevertheless, the formulation still provides a scattering amplitude with the possibility of many interferences. Moreover, it is very easy to distinguish contributions to the different channels (excitation, exchange, and fragmentation) by just monitoring the classical trajectories contributing to these events. This is in contrast to the quantum-mechanical time propagation of an initial state, where it is very difficult to extract from the propagated wave packet the fraction which leads to fragmentation, for instance [7]. To do this exactly, one would have to project the scattered state onto a full three-body continuum wave function which is not known.

For collisions close to threshold, we make two additional approximations which can be justifed within the classical dynamics from which the semiclassical S matrix will be constructed. First, we calculate only the partial wave for total angular momentum $L = 0$. By scaling the phase-space variables (p_i, q_i) of the classical Hamiltonian it can be shown that all partial waves contribute like the S wave in the limit $E \to 0$. Hence, knowledge of the S wave provides the essential information about the cross section. However, the possibility of determining its absolute value is sacrificed. Second, we restrict the calculation to an angle of 180° between the positron and the proton. Formally, this angle is a fixed point of the classical mechanics; i.e., from the initial conditions $\Theta(t_0) = \pi$ and $d\Theta/dt(t_0) = 0$ follows $\Theta(t) = \pi$ for all t. A more physical justification for this approximation considers that the bound orbit of the electron becomes polarized during the approach of the positron, with the geometry of $\Theta = 180°$ being energetically favored. Even if exchange (positronium formation) takes place, the same argument applies now to the positronium which is polarized by the proton while receding from it. The most convincing argument for these approximations close to threshold comes from the excellent agreement of the theoretical and experimental cross sections for ionization of hydrogen by *electron* impact [8].

The approximations reduce the system to two degrees of freedom, which might be taken as the electron-positron (r_1) and electron-proton (r_2) distances with the Hamiltonian (atomic units are used unless stated otherwise)

$$H = p_1^2 + \frac{1}{2}p_2^2 - p_1 p_2 - \frac{1}{r_1} - \frac{1}{r_2} + \frac{1}{r_1 + r_2}. \qquad (1)$$

In the "one-dimensional" world, a cross section has the form of a probability, directly related to the S matrix. The initial bound state appears as a classical Kepler orbit in the coordinate r_2 with energy ϵ'. The semiclassical amplitude for inelastic scattering can be cast into the form [9]

$$S_{\epsilon,\epsilon'}(E) = N^{-\frac{1}{2}} \sum_{\text{cl.traj.}} \left|\frac{\partial r'}{\partial \epsilon}\right|_{\epsilon'}^{\frac{1}{2}} \exp\left(\frac{i\Phi}{\hbar} - \frac{i\nu\pi}{2}\right), \qquad (2)$$

where N is a normalization constant to ensure probability conservation [9]. Equation (2) is similar to Miller's "classical S matrix" from which it can be derived [11]. The sum runs over all classical trajectories which describe the inelastic process under consideration. The classical probability of finding such a trajectory is measured by $N^{-1}\partial r'/\partial\epsilon$. Each trajectory accumulates a phase, which is defined by the classical action $\Phi(\epsilon,\epsilon',E) = \int q_1 dp_1 + \int q_2 dp_2$ and a contribution of $\nu\pi/2$ from caustics along the trajectory [14]. The trajectories connect, for a given total energy E, the asymptotic initial condition of a free positron at a remote position r' and a bound electron of energy ϵ' with the final state characterized by the energy ϵ of the electron. A negative ϵ describes an excitation process, positronium formation is indicated by $\epsilon \geq E$, and the interval $0 < \epsilon < E$ corresponds to fragmentation. Note, however, that some care is needed to extract the electron energy from the asymptotic behavior of the trajectories since the momenta p_i must be expressed in the Jacobi coordinates appropriate for each inelastic final channel.

In the case of fragmentation the action Φ provides the quantum-mechanical form of the logarithmic phase for a three-body Coulomb state in the continuum as derived by Peterkop [10] without imposing any boundary conditions explicitly. However, as will be seen later, the phase is not relevant for threshold ionization.

To determine the scattering amplitude we have to find all trajectories that contribute to the sum in Eq. (2). This can be accomplished by scanning the initial conditions $r'_0 + r'$ with a fixed ϵ' until a trajectory leads to the desired final energy ϵ for the electron. The distance r'_0 is abritrary, but large enough so that the result is independent of r'_0. One finds that only a *single* trajectory with a well defined r' fulfills a set of boundary conditions ϵ, ϵ'. This can be seen from Fig. 1, where the energy of the asymptotically free positron or proton is shown as a function of r' at a given total energy of $E = 2.7$ eV. The plot can be interpreted as a continuous energy transfer from the positron to the proton with increasing r'.

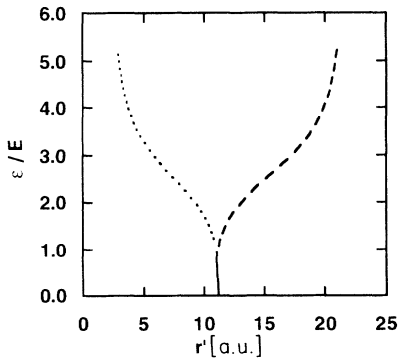

FIG. 1. Energy ϵ of the asymptotically free motion normalized to the total energy $E = 2.7$ eV as a function of the position 100 a.u.$+r'$ of the initially free positron. The dotted line indicates excitation (free positron), the full line fragmentation (the energy of the positron is plotted), and the dashed line positronium formation (kinetic energy of the proton relative to positronium is plotted).

Beginning at the left corner the decreasing energy of the free positron towards greater r' indicates an increasingly excited hydrogen atom as the result of the collision. At some r' the electron-proton motion has gained enough energy during the collision to break the binding so that all three particles are free (solid line). When more energy is transfered to the proton and correspondingly less energy remains for the positron, the momenta of the electron and the positron become comparable and positronium is formed (the center-of-mass energy of the proton with respect to the positronium is shown as a dashed line). Towards large r' the free proton gains successively higher energy.

Figure 2 gives the information of Fig. 1 in a different format, as a function of the total energy E. With only one trajectory contributing to the differential cross section, the phase becomes irrelevant in Eq. (2), which reduces to the purely classical expression

$$P_\epsilon(E) = |S_{\epsilon,\epsilon'}(E)|^2 = \left|\frac{\partial r'}{\partial \epsilon}\right|_{\epsilon'} N^{-1}. \qquad (3)$$

The total cross section is then simply proportional to the intervals of r' for which a certain process, for instance fragmentation, happens:

$$P_{frag}(E) = \int_{\{frag\}} P_\epsilon(E) d\epsilon = N^{-1} \int_{\{frag\}} \left|\frac{\partial r'}{\partial \epsilon}\right|_{\epsilon'} d\epsilon = \frac{\Delta r'_{frag}}{N}. \qquad (4)$$

The intervals $\Delta r'$ and the normalization

$$N = \Delta r'_{frag} + \Delta r'_{\text{PF}} + \Delta r'_{exc} \qquad (5)$$

can be read off directly from Fig. 2. The relative probabilities $P_x(E) = \Delta r'_x/N$ are shown in Fig. 3. It is already clear from Fig. 3 that positronium formation is the dominant contribution to ionization close to the fragmentation threshold. This explains Temkin's conclusion that ionization has a constant cross section at threshold. More interesting is the fragmentation cross section. Our result confirms the power law $\sigma \propto E^{2.65}$ as calculated by Klar

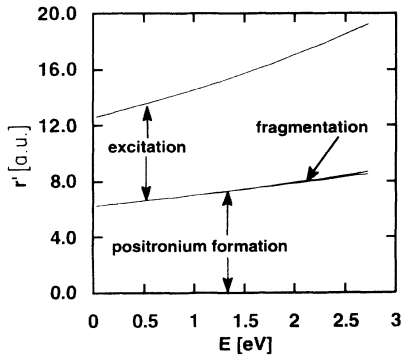

FIG. 2. The initial values r' leading to different inelastic scattering events as a function of total energy.

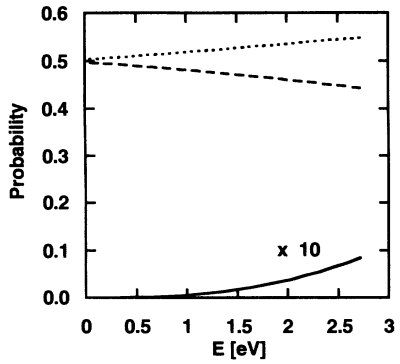

FIG. 3. Relative probabilities for fragmentation (solid), excitation (dotted), and positronium formation (dashed).

from the Wannier theory.

Note that the total probabilities for excitation-positronium formation do not take into account the discrete nature of the bound states of hydrogen-positronium. An obvious but probably not the best way to implement the discrete nature of the quantum states would lead back to Miller's method to define state-to-state ($n' \to n$) transition probabilities and sum over them, $P_{exc}(E) = \sum_n P_{nn'}(E)$ where $n' = 1$ refers to the ground state, the only relevant initial state in the present context. However, it is *a priori* not certain if the *total* excitation yield is approximated better or worse by this procedure than by the nonquantized integral $P_{exc}(E)$ of Eq. (4). This question is beyond the scope of the present paper and will be addressed from a more general perspective of semiclassical methods in future work.

The directly accessible quantity in the experiment [15] is the ratio between the fragmentation and the total ionization

$$R(E) = \frac{P_{frag}(E)}{P_{frag}(E) + P_{\rm PF}(E)} = \frac{\Delta r'_{frag}}{\Delta r'_{frag} + \Delta r'_{\rm PF}}, \quad (6)$$

which is shown together with $P_{frag}(E)$ in Fig. 4. The ratio $R(E)$ follows quite accurately the power law $R(E) = cE^d$ with $c = 1.25 \times 10^{-3}$ and $d = 2.67$. As can be seen from Fig. 4, we predict a ratio R of 2% at 3 eV excess energy. The good fits by a power law as high as 3 eV above threshold indicate that the threshold region extends to higher energies for positron-hydrogen scattering than for electron-hydrogen scattering where a structural change in the differential fragmentation probability $P_\epsilon(E)$ limits the threshold region to roughly 3 eV [8]. While equal energy sharing $\epsilon = E/2$ among the two electrons is most likely below 3.3 eV, the preferred energy sharing for higher energies is a fast (projectile) electron and a slow (ejected) electron. Obviously, this transition cannot occur in positron-hydrogen scattering, where the energy sharing between the proton and the positron is always monotonic. Hence, there is no sudden transition between threshold and nonthreshold regions, and it can be expected that the total cross section is well represented with a power law for relatively high energies. The good quantitative agreement with the Wannier threshold theory is not a consequence of the collinear approximation, although the Wannier theory is also formulated for $\Theta = 180°$. This may be seen in comparison with electron-hydrogen scattering where the semiclassical calculation with the same collinear approximation agrees quantitatively with the Wannier theory only in the limit $E \to 0$ [8].

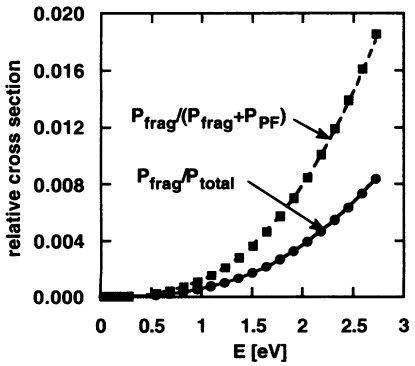

FIG. 4. The fragmentation probability (circles) and the ratio $R(E) = P_{frag}/(P_{frag} + P_{\rm PF})$ (squares), see text. The lines represent fits with a power law $P(E) = aE^b$ (solid) and $R(E) = cE^d$ (dashed), where $b = 2.65$ and $d = 2.67$.

In conclusion the semiclassical analysis has shown that positron-hydrogen scattering close to threshold is a classical process in the sense that only a single trajectory contributes to the differential cross section. Hence, no interference effects occur. The situation is similar to the *two*-body Coulomb scattering. As is well known, the Rutherford scattering cross section can be obtained classically or quantum mechanically. The semiclassical analysis reveals that only a single trajectory contributes to the differential cross section [16], so that the classical and semiclassical results are identical. The same situation is found in the present case of three-body Coulomb scattering: A single trajectory contributes to the differential cross section, so that the results presented here are, apart from the initial bound state of hydrogen, completely classical.

Although the present work is only a calculation for two degrees of freedom, sufficient to cover the relevant dynamics close to threshold, the concept of semiclassical Coulomb scattering is by no means limited to one or two degrees of freedom. In fact, certain technical aspects, like the Coulomb singularity, are even easier to handle in the full three-dimensional space (six degrees of freedom) simply, because the singularity is never hit directly. All trajectories but a set of measure zero have a finite two-body angular momentum which creates an effective centrifugal barrier preventing the collapse into the singularity.

Semiclassical scattering is conceptually most attractive for long-range potentials. While traditional scattering approximations need to resort to special techniques in the case of Coulomb or dipole interactions, the semiclassical theory does not need to be modified for these cases. Moreover, it is not necessary to provide a quantum-

mechanical three-body continuum state for fragmentation, which is very difficult. Instead, one simply adds up the contributions from trajectories which lead to fragmentation. To some extent semiclassical scattering theory and traditional quantum approximations are complementary: Where the quantum approach is relatively simple (excitation-exchange) the semiclassical method requires more effort. Where the quantum approach is very difficult, namely for fragmentation at low and intermediate energies, the semiclassical theory as presented here finds its most natural application.

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