# Threshold laws and reaction zone dynamics of three-body Coulomb breakup

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Wannier theory is critically reexamined and compared with semiclassical *S*-matrix theory, which serves as a reference calculation. We find that for certain situations classical half-collision calculations with a fixed reaction zone radius strongly differ from the results of a full *S*-matrix treatment even at energies very close to threshold. By giving a parameter-free description of an energy-dependent reaction zone radius we take the initial state more accurately into account in the half-collision approach. This extension produces results for ionization probabilities which are in excellent agreement with the full-collision semiclassical *S*-matrix theory. [S1050-2947(99)09011-3]

## I. INTRODUCTION

In his seminal paper on electron-impact ionization Wannier [1] introduced two key assumptions in his description. (1) The quasiergodic hypothesis: the electrons initially have an approximately uniform distribution in phase space about the Wannier saddle point at a hypersphere of radius $R_b$. (2) No initial-state dependence: the initial volume of phase space at the hypersphere $R_b$ remains constant and energy independent. We examine here the validity of these assumptions by comparing full- and half-collision calculations.

We recently studied electron-impact ionization of a system which consists of an electron bound to a nucleus of fractional charge $Z$ [2] using semiclassical *S*-matrix theory [3,4]. Such a system serves as a model for realistic three-body Coulomb processes involving a fractional charge ratio between the central particle and the wing particles (the latter we take to have equal masses and charges). Single ionization of $Be^{3+}$ in a collision with a $Be^{4+}$ ion is an example of a system with charge ratio $Z = 1/4$ which should also be experimentally accessible. We demonstrate in this Brief Report that the analysis of systems with fractional charge gives insight into the understanding of the ionization dynamics of three-body Coulomb systems. In particular, it elucidates the merits and limitations of the Wannier description [1].

When we calculated ionization cross sections we found that for a range of fractional values of $Z$ the cross sections do not follow the Wannier power law even in the threshold regime of very low excess energy $E$ where the saddle-point dynamics is expected to be valid [2]. Dependencies on the choice of the target atom and discrepancies with Wannier theory have also been noticed in the context of the spin asymmetry parameter near threshold for hydrogen [5–7]. The investigations in these papers pointed towards the importance of going beyond the Wannier description and to take the reaction zone dynamics, where the three particles are close to each other, more accurately into account.

In Sec. II we put to a critical test one of the underlying assumptions of Wannier theory. We first test how well justified the *quadratic expansion* of the three-particle potential around the Wannier ridge is. To that end we compare Wannier theory with a *numerical half-collision calculation*. At this stage we keep the second major ingredient of Wannier theory untouched, namely the *equal distribution* of initial conditions of trajectories in phase space at a *fixed* small interparticle distance characterized by the hyperradius of the system [1].

In Sec. III we also drop the assumption of a fixed hyperradius from which trajectories start on their way to ionization. We discuss and justify why it is more appropriate to introduce an energy dependence for the hyperradius. This effectively corresponds to an energy dependence of the initial state in a half-collision treatment, a fact that may surprise one at first. The benchmark against which our results are compared to is the results calculated with the semiclassical *S*-matrix method [3,4], briefly described and related to the Wannier approach in Sec. IV. This theory describes electron-impact ionization as a *full-collision process* and takes the *full* three-particle potential numerically into account. Sec. V is devoted to a discussion and comparison of the different approaches.

## II. RIDGE PROPAGATION BEYOND WANNIER THEORY

In Wannier's analysis of the ionization process the classical equations of motion are written in terms of the hyperspherical coordinates $R = \sqrt{(r_1^2 + r_2^2)}, \tan\alpha = r_2/r_1$ and $\theta_{12}$, where $r_1$ and $r_2$ are the distances of the electrons from a nucleus of charge $Z$ and $\theta_{12}$ is the angle between the electrons. He deduced that the trajectories that are important for ionization near threshold are those in the vicinity of the saddle point of the potential. Linearizing the equations of motion about the saddle point the solution can be written as

$$\beta = \frac{\pi}{4} - \alpha = C_1 R^{-\mu/2 - 1/4} + C_2 R^{\mu/2 - 1/4}, \quad (1)$$

where $\mu = \frac{1}{2}[(100Z - 9)/(4Z - 1)]^{1/2}$ and $\zeta = \mu/2 - 1/4$ is the Wannier exponent [1].

The quantity $C_2$, which enters as an integration constant in the solution, characterizes the initial conditions of a trajectory in phase space on a hypersphere of constant, energy-independent, hyperradius $R_b$. $\Delta C_2$ is the length of the interval of values for $C_2$ which leads to ionizing trajectories. It depends on the energy and is proportional to $E^\zeta$. The Wannier ionization probability is given by
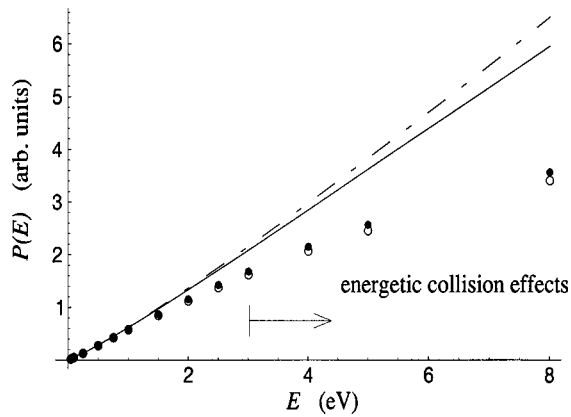
FIG. 1. Ionization cross sections for $Z=1$. Dashed line: Wannier power law. Solid line: numerical half-collision result with $R_b$ constant (1 a.u.). The solid circles are the numerical half-collision result with an energy dependent $R_b(E)$ as described in Sec. III. The open circles are the full-collision semiclassical $S$-matrix result.

$$P_{\text{wan}} \sim \Delta C_2 \sim (R_b E)^{\zeta}. \tag{2}$$

To test the energy range over which the Wannier result is valid we first drop the quadratic approximation for the potential and calculate ionization probabilities numerically as a half-collision process, incorporating the full three particle potential. Trajectories are started at a fixed hyperradius $R_b$ with an ergodic distribution of initial conditions on the hypersphere. The ratio of ionizing trajectories is the ionization probability $P_{\text{ion}}$.

Fig. 1 shows the result of such a calculation for hydrogen ($Z=1$). The Wannier threshold law (2), which determines the threshold behavior up to a proportionality constant, is adjusted to the numerical result at the lowest numerical data point. There is very good agreement up to an energy of approximately $E=2.5$ eV with the numerical result becoming lower than the Wannier power law at higher energies. These differences become more pronounced as $Z$ decreases. At $Z=0.26$ the differences between the numerical result and the Wannier power law become significant already at very low energies (Fig. 2).

We find that a numerical half-collision calculation in the quadratic approximation is in agreement with the numerical calculation with the full potential over the energy ranges of Figs. 1 and 2. The difference with Wannier's power law is due to an additional energy dependence of the initial state which arises as a consequence of the energy-dependent initial hyperradial momentum used in the numerical calculations (as opposed to the $E=0$ momentum employed in formulating the equations of motion in Wannier theory).

### III. ENERGY-DEPENDENT REACTION ZONE RADIUS

So far we have taken the initial hyperradius $R_b$ to be independent of energy $E$ in our numerical half-collision calculations to preserve the spirit of Wannier theory as far as possible. Classically the ergodic distribution of initial conditions on a hypersphere of fixed radius $R_b$ represents the initial state of the three-particle complex in a half-collision treatment before break up. In this section we demonstrate
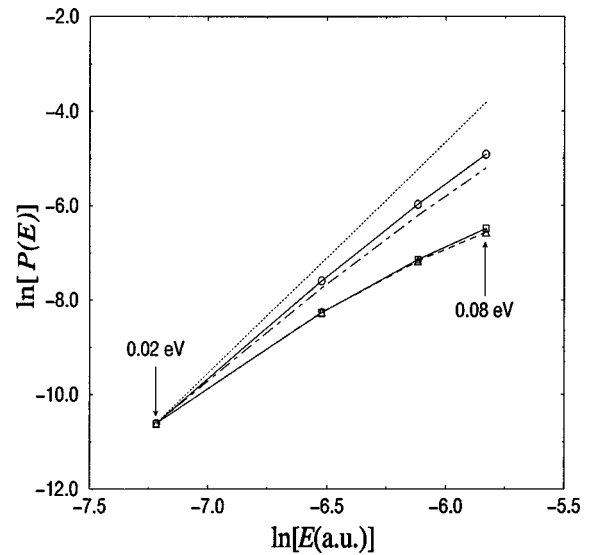


FIG. 2. Ionization cross sections for $Z=0.26$. Dotted line: Wannier power law. Dot-dashed line: numerical half-collision result with $R_b$ constant. The solid line with square data points is the numerical half-collision result with energy-dependent $R_b(E)$. The solid line with circular data points is expression (5) with energy-dependent $R_b(E)$. The dashed line with triangular data points is the $S$-matrix result.

that a more accurate half-collision description requires the introduction of an energy dependence for the reaction zone radius $R_b$.

To this end we performed a numerical full-collision calculation in the collinear configuration where the electron interaction is replaced by $1/(r_1+r_2)$ [2] and which has been demonstrated to be the relevant geometry near threshold [4]. $R_b(E)$ is defined as the radius where one of the electrons hits the nucleus for the last time before the outward motion of both electrons begins. $R_b(E)$ depends on the full-collision trajectory under consideration and decomposes it into its incoming and outgoing part.

Figure 3 demonstrates the energy dependence of $R_b(E)$ for two trajectories with different total energies which asymptotically lead to an equal energy sharing between the electrons ($\alpha \to \pi/4$ as $R \to \infty$) for the case $Z=1$. At a fixed total energy $E$ we have chosen $R_b(E)$ to be the radius of the leading Wannier trajectory which converges towards the ridge as depicted in Fig. 3. This choice seems reasonable since in the Wannier picture it is the motion of outgoing trajectories in the vicinity of the ridge ($\alpha \approx \pi/4$) which determines the ionization probability. Figure 4 shows the thus determined reaction zone radius $R_b(E)$ as a function of total energy for the system with nuclear charge $Z=1$.

The effect of a variation of $R_b$ on the ionization probability can be understood in the following way: If a trajectory starts at a smaller value of $R_b$ it will have to travel a further distance along the potential ridge before reaching the radius $R_c$ that characterizes the boundary between the Coulomb zone and the free zone beyond which trajectories can be counted as ionized. This means that if two trajectories at the same energy have different values of $R_b$ then the trajectory that corresponds to the smaller value of $R_b$ will have less chance of ionizing since its survival probability on the ridge will be smaller.
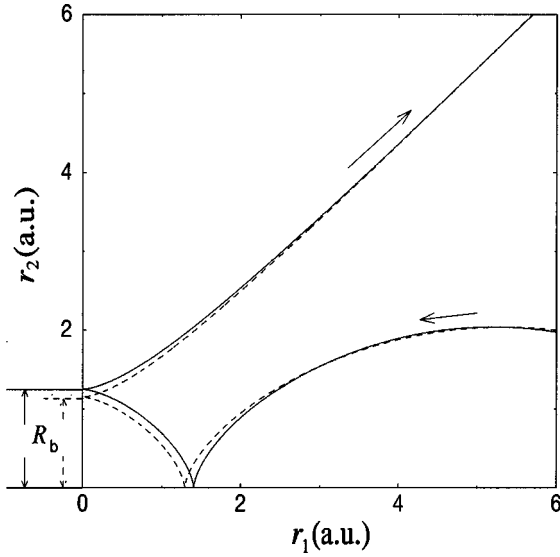
FIG. 3. Reaction zone radius $R_b$ for two ionizing trajectories which correspond to an equal energy sharing between electrons for $Z=1$ at $E=0.05$ eV (solid line) and $E=2.5$ eV (dashed line).

## IV. IONIZATION PROBABILITIES

Before comparing an extended version of Wannier theory, which takes the energy dependence of $R_b$ into account with semiclassical $S$-matrix theory, a few words must be said about normalization of ionization probabilities. The probability for electron-impact ionization in semiclassical $S$-matrix theory is given by [3,4]

$$P_{\mathrm{scs}}(E) = \frac{1}{\mathcal{R}(E)} \int_0^E \mathrm{d}\varepsilon \left| \frac{\mathrm{d}r'}{\mathrm{d}\varepsilon} \right| = \frac{\Delta r'_{\mathrm{ion}}}{\mathcal{R}(E)}, \qquad (3)$$

where $\varepsilon$ denotes the asymptotic energy of one of the electrons after ionization and $r'$ is the initial distance of the incoming electron to the nucleus. The classical deflection function $|\mathrm{d}r'/\mathrm{d}\varepsilon|$ gives the functional dependence between the initial-state parameter $r'$ and the final-state parameter $\varepsilon$.
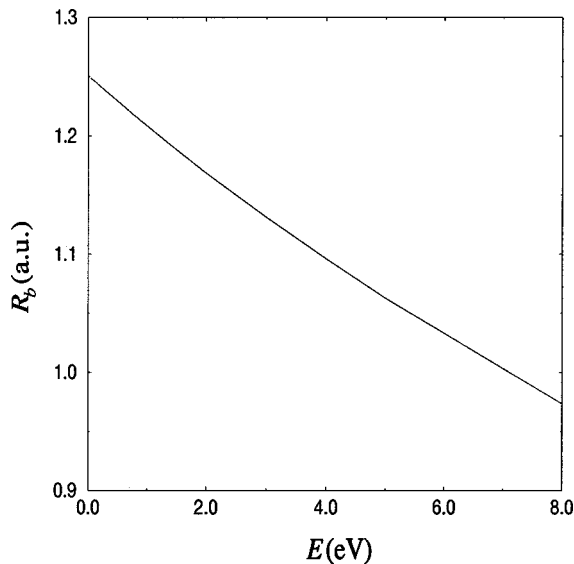


FIG. 4. Energy dependence of the reaction zone radius $R_b$ for a system with nuclear charge $Z=1$.

$\Delta r'_{\mathrm{ion}}$ is the interval of initial conditions which leads to ionizing trajectories. The ionization probability (3) is normalized with respect to the period $\mathcal{R}(E)$ of the deflection function. $\mathcal{R}(E)$ is proportional to $\sqrt{E+Z^2/2}$ and is the interval of initial conditions $r'$ over one period of oscillation of the initially bound electron. The distribution of initial conditions in $\mathcal{R}(E)$ is taken to be uniform.

In analogy the deflection function in Wannier theory can be defined as the dependence of the asymptotic value of $\varepsilon$ on $C_2$ which characterizes the initial condition of outgoing trajectories on the hypersphere $R_b$. Integration over the ionization interval leads to the Wannier result

$$P_{\mathrm{wan}}(E) \sim \int_0^E \mathrm{d}\varepsilon \frac{\mathrm{d}C_2}{\mathrm{d}\varepsilon} = \Delta C_2. \qquad (4)$$

The Wannier probability $P_{\mathrm{wan}}(E)$ is given up to a normalization constant. The problem we are faced with is that it is not as easy to determine the allowed interval of values for $C_2$ as it is for $r'$.

Our crucial assumption now is that the equal distribution of initial conditions in $\mathcal{R}(E)$ in the *full-collision* $S$-matrix approach translates into an equal distribution of initial conditions on the reaction zone radius $R_b(E)$. We thus modify Wannier theory in a way to allow for an energy-dependent reaction zone radius as described in the previous section but keep the quasiergodic hypothesis of uniform distribution of initial conditions untouched. We are then allowed to write the ionization probability in what we will call an extended Wannier theory as

$$P_{\mathrm{ext}}(E) = \frac{[R_b(E)E]^\xi}{\mathcal{R}(E)}. \qquad (5)$$

## V. COMPARISON WITH $S$-MATRIX THEORY

We now compare the extended Wannier approach with the result from $S$-matrix theory. The semiclassical $S$-matrix treatment demonstrates that saddle-point dynamics is valid up to approximately 2.5 eV for $Z=1$. However, when $R_b$ is fixed in a half-collision approach there is not agreement over this entire energy range (Fig. 1). The energy dependence of $R_b$ is now incorporated into a numerical half-collision calculation for $Z=1$. For each energy we set $R_b$ to the calculated value as described in Sec. III and evaluate the ionization probability. We have seen in Sec. II that the numerical half-collision calculation is in very good agreement with the Wannier power law up to 2.5 eV. The numerical result with energy-dependent $R_b$ thus coincides with expression (5) over this energy range. The agreement with a full-collision treatment is also excellent. Above $E=2.5$ eV a difference between the half- and full-collision methods becomes apparent and is due to the differential cross section changing its form to a preferred unequal energy sharing so that Wannier theory, even in its modified version, can no longer be expected to apply [3].

When $Z=0.288$ the cross section calculated with semiclassical $S$-matrix theory shows a surprising behavior; the slope on a logarithmic graph is larger than the Wannier power law. This type of cross section only exists for a small range of values of $Z$ [2]. At low energies a numerical half-

collision calculation with fixed $R_b$ is in good agreement with the Wannier power law. In Fig. 5 we see that expression (5) with an energy dependent $R_b(E)$ agrees well with the $S$-matrix calculation. At the low energies plotted the normalization $\mathcal{R}(E)$ has negligible effect on the result, demonstrating that the large deviation from the Wannier power law is due entirely to the reaction zone dynamics. In terms of $R_b$ it is noticed that in these cases $R_b$ increases when the energy is increased (which is opposite of the dependence for $Z=1$, see Fig. 4). Thus the way the actual ionization probability deviates from the Wannier result can be put into direct relation with the energy dependence of $R_b(E)$.

At very low energies near $E=0.02$ eV the cross section for $Z=0.26$ does not follow the Wannier power law. We checked that the deviation of the $S$-matrix result from the Wannier law happens already in an energy regime where an equal distribution of energy among the escaping electrons is still the most probable process. Figure 2 shows separately the effects of including $R_b(E)$ and performing a numerical calculation (which now introduces a significant correction to the Wannier power law over the energy range of the plot). When both corrections are made together (solid line with square data points) we observe excellent agreement with the $S$-matrix result.

## VI. CONCLUSION

We have found three-body Coulomb systems where the ionization probability deviates from Wannier's prediction at energies even very close to threshold. We identified these deviations as arising from an energy dependence of the reaction zone radius $R_b(E)$ which enters in half-collision approaches. We provided a simple, parameter-free, description to determine the energy dependence of $R_b(E)$. For energy regimes where the ionization probability is dominated by ridge propagation and Wannier theory is applicable, our extended Wannier approach, given by Eq. (5) with an energy-dependent reaction zone radius $R_b(E)$, gives results that are in excellent agreement with full-collision $S$-matrix theory for
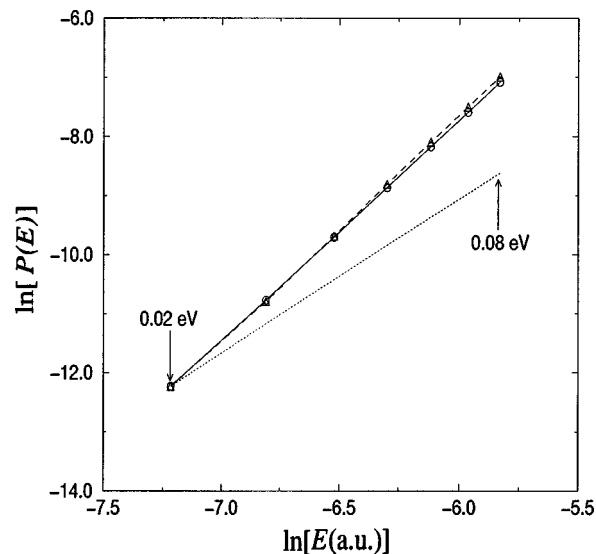


FIG. 5. Ionization cross sections plotted on a double logarithmic scale for $Z=0.288$. The dotted line is the Wannier power law. The solid line with circular data points is expression (5) with energy-dependent $R_b$. The dashed line with triangular data points is the semiclassical $S$-matrix result.

a range of $Z>1/4$. However, as one approaches $Z=1/4$ it becomes important to numerically incorporate the full energy-dependent dynamics already at very small energies. In contrast to Wannier theory, which uses only $E=0$ trajectories [see Eq. (1)] a numerical half-collision treatment takes the *energy dependence of the ionization dynamics* into account, and leads to results that again are in exellent agreement with full-collision $S$-matrix theory for $Z$ close to $1/4$.

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