Classical threshold behaviour in a (1+1)-dimensional model for double ionization in strong fields

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Abstract

Building on insights into the classical pathways to double ionization in strong laser fields, we here propose a (1+1)-dimensional model that captures essentials of the 3D potential landscape and allows efficient studies of the process in reduced dimensions. The reduction to one degree of freedom for each electron is obtained by confining their motion to lines at an angle of \(\pi/6\) with respect to the field axis; the justification for this choice is that upon variation of the electric field the Stark saddles move along the same lines. In this way, we obtain a low-dimensional representation in which symmetric electron escape is possible. As a demonstration of the advantages of this model, we numerically confirm the equivalent of the Wannier threshold behaviour for constant electric field and identify several classes of trajectories that can contribute to the ionization process.

Introduction

Analysing the dynamics of two-electron systems remains a challenge because of the high dimensionality of the configuration space, especially when highly excited states are involved, as in the case of strong field double ionization. The Taylor group managed to obtain results for a full (3+3)-dimensional representation, albeit mostly at short wavelength [1, 2]. (1+1)-dimensional models with both electrons aligned along one axis [3–6] are attractive (as reflected in a large number of publications based on this model), but physically flawed since the electron repulsion prevents an escape in the experimentally observed subspace of equal momenta [7–13]. Among the alternatives that have been considered are models where the centre of mass of the electrons is confined to move along the axis [14]: they might be classified as (1.5+1.5) dimensional, since the position of an electron along the field axis qualifies as a full degree of freedom and the perpendicular one, being shared with the other electron, as half a degree of freedom. It is our aim here to present and analyse a model with further constraints on
the dynamics; the model nevertheless captures several essential features of the full dynamics and allows efficient simulations.

The model is suggested by our previous analysis of the classical pathways to non-sequential double ionization in strong laser fields [15–17]. We found that the observed symmetric escape can be explained by the escape over a symmetrically arranged saddle. The origin of the saddle can be traced to the case of a single electron in an external field, where it is located at the position where Coulomb attraction to the centre and the pulling by the field cancel each other. For two electrons their mutual repulsion also has to be counterbalanced by the Coulomb attraction from the centre: the saddle configuration then becomes one of two electrons located symmetrically with respect to the field axis. As the field changes, the saddle moves along lines that keep a constant angle with respect to the polarization axis. Confining the electrons to run along 1D tracks that pass through the saddles gives a model for (1+1)-dimensional electron dynamics that has a potential landscape topology very similar to that for electrons in the full 3D case. While the potential turns out to be very similar to the so-called aligned-electron model [3–6], it has one significant difference: since the electron tracks separate as they move away from the nucleus electron repulsion diminishes as the electrons go out. Thus, the diagonal, where the two electron coordinates are equal, is accessible and not, as in the aligned model, suppressed by electron repulsion. This allows us to mimic a key feature of the observed double ionization dynamics, namely the preference for symmetric electron escape [7–13].

In the present paper, we analyse the model classically for the case of a static electric field. The static field forms a local maximum in the potential energy (that corresponds to the saddle in the 3D case [15]) close to which simultaneous escape of electrons takes place. If the energy of the system equals the energy of the stationary point only purely symmetric electron motion leads to the simultaneous escape. For higher energy, some deviations from the symmetric motion are allowed. The stability analysis of the saddle point in the full 3D case allowed us to predict the dependence of the classical cross section for the process on energy close to the threshold [17], i.e. to obtain the Wannier threshold law [18–20] in the presence of the external field. However, the results of the local analysis were difficult to verify in 3D numerical simulations. The key features of the 3D potential are present in our (1+1)-dimensional model that allows us to also obtain the threshold law and moreover verify it in numerical simulations.

The model

We begin with a reminder of the saddle configurations in the symmetric subspace in the 3D case [15–17]. Assume the external electric field points in the z-direction and the electrons are labelled $i = 1, 2$ with positions $\mathbf{r}_i = (x_i, y_i, z_i)$. Then the Hamiltonian, in atomic units, is

$$H = \sum_{i=1}^{2} \left\{ \frac{\mathbf{p}_i^2}{2} - \frac{2}{|\mathbf{r}_i|} - F z_i \right\} + \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|}. \tag{1}$$

Let the electrons move in the x-z-plane, symmetric with respect to the field axis. Then, their positions are $(x, 0, z)$ and $(-x, 0, z)$ and the potential energy becomes

$$V = -\frac{4}{\sqrt{x^2 + z^2}} + \frac{1}{2|x|} - 2Fz. \tag{2}$$

This potential energy has a saddle at $x_s = 3^{1/4}/(2\sqrt{F})$, $z_s = 3^{3/4}/(2\sqrt{F})$, with energy $-3^{3/4}2\sqrt{F}$. Note that if we allow for the variation of the field strength (like, e.g., in a laser field), the saddle moves along lines with $z_s/x_s = \sqrt{3} = \text{const}$. Because simultaneous electron escape takes place in the vicinity of the saddle, the idea is then to assume that the electrons
move in a plane, \( y_i = 0 \), with coordinates constrained exactly by this relation, \( z_i^2 = 3x_i^2 \). This leaves only one degree of freedom for each electron, called \( r_1 \) and \( r_2 \):

\[
\begin{align*}
  x_1 &= -\frac{1}{2}r_1 \\
  z_1 &= \frac{\sqrt{3}}{2}r_1 & \text{and} & \quad x_2 &= \frac{1}{2}r_2 \\
  z_2 &= \frac{\sqrt{3}}{2}r_2.
\end{align*}
\]

The Hamiltonian becomes

\[
H = \frac{p_1^2 + p_2^2}{2} - \frac{2}{|r_1|} - \frac{2}{|r_2|} + \frac{1}{\sqrt{(r_1 - r_2)^2 + r_1r_2}} - \frac{F\sqrt{3}}{2} (r_1 + r_2).
\]

The Hamiltonian (4) defines our (1+1)-dimensional model and in the following we restrict ourselves to the description of the two-electron system within this model.

When the external field is present, the potential energy in (4) has a saddle located at

\[
r_1 = r_2 = r_s = \frac{3^{1/4}}{\sqrt{F}}.
\]

with energy

\[
V_s = -3^{3/4}2\sqrt{F}.
\]

The equipotential contours for \( F = 0.02 \) are plotted in figure 1; the stationary point near \( r_1 = r_2 \approx 9.3 \) is clearly visible. There is a symmetric subspace in the full phase space of the (1+1)-dimensional system and the stationary point lives in this subspace. That is, if initial conditions are chosen symmetrically, i.e. \( r_1 = r_2 \) and \( p_1 = p_2 \), the electron motion remains symmetric in time evolution. Trajectories that pass close to the stationary point and sufficiently close to the symmetric subspace lead to simultaneous electron escapes.

**Wannier threshold law**

The potential energy in (4) possesses a stationary point located at (5), i.e. in the symmetric subspace of the system. The stability analysis of the stationary point in the full phase space allows us to determine the behaviour of the cross section for simultaneous electron escape close to the threshold [17]. There are two Lyapunov exponents of the point. The first,

\[
\lambda_r = 3^{1/8}F^{3/4},
\]
with the eigenvector in the symmetric subspace, corresponds to a simultaneous motion of the electrons in the same direction away from the nucleus. Borrowing terminology from chemical reactions, we call this subspace the reaction coordinate. Because of the repulsion between electrons, there is an additional unstable direction, with Lyapunov exponent

$$\lambda_\perp = \sqrt{\frac{11}{6}} \frac{3^{1/8}}{F^{3/4}},$$  \hspace{1cm} (8)

which enters in the threshold law. If the initial energy of the system equals the stationary point energy only a trajectory living in the symmetric subspace can lead to a simultaneous escape of both electrons. This reduces the dimensionality of the problem and the cross section vanishes. For higher energy some deviations from the symmetric motion are possible, giving a finite volume of initial conditions and a non-vanishing cross section. The dependence of the cross section on energy $\sigma(E)$ close to the stationary point energy $V_s$ can be obtained in the spirit of the Wannier analysis [17–21], resulting in

$$\sigma(E) \sim (E - V_s)^\mu,$$  \hspace{1cm} (9)

with an exponent

$$\mu = \frac{\lambda_\perp}{\lambda_r} = \sqrt{\frac{11}{6}} \approx 1.354.$$  \hspace{1cm} (10)

This is larger than the corresponding exponent in the full 3D case where, for a doubly charged remaining ion, the exponent is 1.292 [17]. The cross section is larger if the exponent is smaller, i.e. if the saddle is crossed more quickly (larger $\lambda_r$) or if the differences from the symmetric motion grow more slowly (smaller $\lambda_\perp$). This cross section exponent is an additional characteristic of the double ionization process.

**Numerical results**

The derivation of the cross section exponent (10) for the simultaneous electron escape is based on the local analysis of the stationary point of the system. One may wonder if the higher order terms can modify the behaviour of the cross section. To test the results of the local analysis, we can perform numerical simulations of the process by integrating the initial value problem for the classical equations of motion. In the 3D case considered in [17] that was quite difficult due to the high dimensionality of the problem. Here, we effectively deal with the three-dimensional phase space and the numerical simulations become feasible.

In order to avoid problems with the Coulomb singularities, we can add cut-offs in the denominator, so that the potential becomes

$$V \equiv -\frac{2}{\sqrt{r_1^2 + 1}} - \frac{2}{\sqrt{r_2^2 + 1}} + \frac{1}{\sqrt{(r_1 - r_2)^2 + r_1 r_2 + 1}} = \frac{F}{2} \sqrt{3} (r_1 + r_2).$$  \hspace{1cm} (11)

The cut-offs slightly change the prediction for the threshold exponent which now equals $\mu = 1.357$ (for $F = 0.02$). We have run trajectories with initial conditions chosen microcanonically for different energies $E$ above the threshold energy $V_s$ but with an additional requirement that they have to lie on the surface $r_1 + r_2 = 0$. We deal with an open system and the condition $r_1 + r_2 = 0$ ensures that the trajectories start in the vicinity of the nucleus. In figure 2, the number of trajectories leading to simultaneous electron escape together with the numerical fit of the function (9) versus energy are shown. The fitted value of the cross section exponent is $1.383 \pm 0.031$ which agrees with the theoretical prediction.

In figure 2, we have included only trajectories leading to simultaneous escape of both electrons. However, it is possible that the first electron ionizes by passing close to the stationary
Figure 2. Number of ionized trajectories (circles with statistical error bars) versus energy above the threshold energy, i.e. the energy of the maximum of the potential (11), corresponding to $F = 0.02$ ($1.5 \times 10^6$ trajectories have been integrated to obtain each point). Solid line is the fit of (9) to the numerical data that results in $\mu = 1.383 \pm 0.031$.

Figure 3. (a) Trajectories (dashed lines) belonging to the separatrix that divides the phase space into areas of simultaneous electron escape and double escape with a single revisit of the nucleus by one of the electrons; solid lines are examples of trajectories leading to simultaneous electron escape. (b) Trajectories (dashed lines) belonging to the separatrix that divides double ionization trajectories with single and double revisit of the nucleus; solid lines are examples of trajectories leading to double ionization with a single revisit of the nucleus by one of the electrons. All trajectories correspond to: $F = 0.02$, energy $E = V_s + 0.1$, symmetric initial momenta $p_1 = p_2$ and positions lying on a circle, i.e. $r_1 = (r_s/2) \cos \alpha$ and $r_2 = (r_s/2) \sin \alpha$.

point while the other one is returned and after revisiting the nucleus ionizes too. Actually, there is a separatrix that divides the phase space into areas corresponding to simultaneous escapes and escapes with a single revisit of the nucleus. The separatrix consists of trajectories where the first electron escapes while the other one approaches a single electron Stark saddle and loses its kinetic energy. Finally, when the first electron is gone, the other electron remains at the single electron saddle with no kinetic energy. In figure 3, there are examples of ionized trajectories and trajectories belonging to the separatrix. All trajectories in figure 3 correspond to: $F = 0.02$, energy $E = V_s + 0.1$, symmetric initial momenta $p_1 = p_2$ and positions lying on a circle, i.e. $r_1 = (r_s/2) \cos \alpha$ and $r_2 = (r_s/2) \sin \alpha$. With these conditions
if $|\pi/4 - \alpha|$ is smaller than about 0.0154\pi simultaneous escape takes place. For greater $|\pi/4 - \alpha|$ but smaller than about 0.0155\pi, the second electron revisits the nucleus and then escapes. At $|\pi/4 - \alpha| \approx 0.0155\pi$, another separatrix appears that separates double ionization trajectories with single and double revisit of the nucleus. This separatrix (see figure 3) consists of trajectories where the second electron after revisiting the nucleus approaches the single electron Stark saddle losing its kinetic energy so that finally it stands on the saddle. With further increase of $|\pi/4 - \alpha|$, the number of revisits increases quickly until the returning electron has too little energy to cross the single electron saddle even if the first electron is gone.

Conclusions

The analysis of pathways to non-sequential double ionization of atoms in strong fields [15–17] allows us to propose a (1+1)-dimensional model of the process. In the present paper, we analyse the model in the case of a static electric field. The Wannier threshold law for simultaneous electron escape in the presence of the static field is derived and tested numerically. We also identify separatrices that divide the phase space of the system into areas of simultaneous electron escapes and double escapes with a multiple revisit of the nucleus by one of the electrons. In classical mechanics, these different trajectories contribute independently to the double ionization process. In quantum mechanics, one may expect interesting coherence effects resulting from interference of the different paths.

The model is considered classically and for a static external field only. However, quantum calculations of double ionization in strong laser field [22–24] including electron tunnelling, rescattering and subsequent double escape can be performed numerically very efficiently within the model. As we have mentioned in the introduction, the crucial advantage of the model over the well-known aligned-electron model [3–6] is that it does not forbid symmetric simultaneous escapes of electrons that are observed experimentally and cannot be described by the aligned-electron model due to an overestimation of the Coulomb repulsion.

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