Entanglement measures in doubly excited states and nondispersive wave packets in planar helium

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Abstract

We calculate the amount of entanglement for bound and doubly excited singlet states below the second, third and fourth ionization thresholds in planar helium. Furthermore, we investigate the dynamics of entanglement in nondispersive two-electron wave packets generated by the resonant coupling of frozen planet states of helium. We show that it is possible to obtain a two-electron nondispersive wave packet for which the time-average entanglement is greater than for each of the unperturbed coupled states.

1. Introduction

Entanglement is one of the most significant characteristics in the quantum mechanical description of multipartite systems [1] and plays an important role in understanding fundamental phenomena such as quantum correlations [2]. Motivated not only for the interest on the foundations of quantum mechanics but also for the possible technological applications in quantum information, quantum computing [3], quantum cryptography [4], and quantum teleportation [5] there has been an increasing activity in the entanglement properties in atomic systems. While most studies on entanglement in atoms have been focused on bound levels of simplified models [6–11], there is rather few information on the entanglement properties of realistic atomic systems. In this regard, the helium atom enjoys an important place. It is the simplest naturally available atomic species which contains the electron–electron interaction, and, therefore a natural candidate for the investigation of entanglement properties in atoms. Previous investigations have been restricted to singly excited states [9, 12–14]. More recently, entanglement measures have been calculated for doubly excited states (DES) below the second ionization threshold in helium [15, 16]. All these investigations have been restricted to the amount of entanglement in atomic states of the unperturbed atom and, up to our knowledge, there is no information about the dynamics of the amount of entanglement in driven two-electron atoms.

The purpose of the present work is to calculate the amount of entanglement for singlet bound and doubly excited states below the second, third and fourth ionization thresholds in planar helium. Furthermore, we report the first calculations of the dynamics of entanglement in certain two-electron wave packets. We pay special attention to particular doubly excited states of helium called frozen planet states (FPS) which are associated with highly correlated classical configurations [17, 18]. Under near-resonantly periodic driving, FPS transform into nondispersive two-electron wave packets (NDWP) [19–22]. That is quantum objects that propagate without dispersion along the classical periodic orbits of frozen planet configuration for long periods of time [22].

This paper is organized as follows. In section 2, we briefly discuss the spectrum of the unperturbed planar helium, the approach to investigate FPS under periodic driving, and the entanglement measure for our system of two identical fermions. In section 3 we present and discuss the results for the amount of entanglement in bound, doubly excited states and nondispersive wave packets. Finally, section 4 contains the summary, some conclusions and perspectives.

2. Theory

2.1. Unperturbed atom

In the center of mass system within the infinite nucleus mass approximation, the dynamics of a two-electron atom is governed by the following Hamiltonian given in atomic units (a.u.),
where the parameter $\gamma$ characterizes the electron-electron interaction and $Z$ represent the charge of the nucleus (for helium $\gamma = 1$ and $Z = 2$). The positions of the electrons with respect to the nucleus are denoted by $\vec{r}_1$ and $\vec{r}_2$, and $\vec{p}_1$ and $\vec{p}_2$ are their conjugate momenta.

The energy levels in helium are organized in Rydberg series labelled by the principal quantum number $N$ of the inner electron. These series converge to single ionization thresholds, which, in turn, converge to the double ionization threshold. Above the first ionization threshold ($N > 1$), doubly excited states in helium are resonances embedded into the continuum spectra.

We compute the unperturbed eigenstates of planar helium following the *ab initio* method described in [22, 23]; a combination of the complex rotation with a representation of Hamiltonian (1) in parabolic coordinates without adjustable parameters leads to the generalized eigenvalue problem

$$A|\Psi_{i,\theta}\rangle = E_{i,\theta}|\Psi_{i,\theta}\rangle,$$

where $A$ and $B$ are the matrix representations of (1) and of the Jacobian $J = 16r_1r_2r_{12}$ of the coordinate transformation, respectively.

Within the complex rotation method, DES appear with complex eigenvalues $E_{i,\theta} = E_i - i\Gamma_i/2$, where the real part corresponds to the energy $E_i$ of the resonance, and the imaginary part contains the decay rate $\Gamma_i$, which is the inverse of the resonance lifetime.

The eigenvectors $|\Psi_{i,\theta}\rangle$ of the rotated Hamiltonian are normalized for the scalar product

$$\langle \Psi_{i,\theta}|B|\Psi_{i,\theta}\rangle = \delta_{ij},$$

and satisfy the closure relation

$$\sum_i |\Psi_{i,\theta}\rangle \langle \Psi_{i,\theta}| = 1,$$

where $\langle \Psi_{i,\theta}|$ is the transpose of $|\Psi_{i,\theta}\rangle$.

Some observables can be calculated with the help of the projection operator of a real energy state $|\phi_E\rangle$ expressed in terms of the eigenvectors $|\Psi_{i,\theta}\rangle$ of the rotated Hamiltonian [24–26],

$$|\phi_E\rangle = \frac{1}{2\pi i} \sum_i \left\{ \frac{R(-\theta)|\Psi_{i,\theta}\rangle}{E_{i,\theta} - E} \left( \overline{\Psi}_{i,\theta}|R(\theta)\rangle \right) - \frac{R(\theta)|\Psi_{i,\theta}\rangle}{E_{i,\theta} - E} \left( \overline{\Psi}_{i,\theta}|R(-\theta)\rangle \right) \right\},$$

where $R(\theta)$ is the complex rotation operator and $\theta$ the rotation angle. In particular, the product of probability amplitudes $\langle \tilde{r} |\phi_E\rangle \langle \phi_E|\tilde{r}' \rangle$ can be obtained within the single pole approximation [27]. Its expression reads

$$\langle \tilde{r} |\phi_E\rangle \langle \phi_E|\tilde{r}' \rangle \simeq \langle \tilde{r} |R(-\theta)|\Psi_{i,\theta}\rangle \langle \overline{\Psi}_{i,\theta}|R(\theta)\rangle \langle \overline{\Psi}_{i,\theta}|R(-\theta)\rangle \langle \overline{\Psi}_{i,\theta}|R(-\theta)\rangle.$$

Using the relations

$$\langle \overline{\Psi}_{i,\theta}|R(\theta)\rangle \tilde{r} \rangle = \langle \overline{\Psi}_{i,\theta}|R(-\theta)\rangle \tilde{r} \rangle,$$

$$\langle \overline{\Psi}_{i,\theta}|R(-\theta)\rangle \tilde{r} \rangle = \langle \overline{\Psi}_{i,\theta}|R(\theta)\rangle \tilde{r} \rangle,$$

$$\langle \overline{\Psi}_{i,\theta}|R(-\theta)\rangle \tilde{r} \rangle = \langle \overline{\Psi}_{i,\theta}|R(\theta)\rangle \tilde{r} \rangle,$$

equation (6) is written as

$$\langle \tilde{r} |\phi_E\rangle \langle \phi_E|\tilde{r}' \rangle \simeq \langle \tilde{r} |R(-\theta)|\Psi_{i,\theta}\rangle \langle \overline{\Psi}_{i,\theta}|R(-\theta)\rangle \langle \overline{\Psi}_{i,\theta}|R(-\theta)\rangle \langle \overline{\Psi}_{i,\theta}|R(-\theta)\rangle \langle \overline{\Psi}_{i,\theta}|R(-\theta)\rangle,$$

which leads to the electronic density

$$|\phi_E(\tilde{r})|^2 = 2 \text{Re} \langle \tilde{r} |R(-\theta)|\Psi_{i,\theta}\rangle^2.$$

Expressions (10) and (11) seem to be independent of the rotation angle $\theta$ since the backward rotation $\langle \tilde{r} |R(-\theta)\rangle$ of the spatial coordinate compensates the rotation of the state $|\Psi_{i,\theta}\rangle$. However, due to the normalization condition (3) it holds

$$e^{-3i\theta} \int d^4p_J \langle \tilde{r} \rangle |R(-\theta)|^2 = 1,$$

where $\vec{r}$ is the fourth dimensional position vector in parabolic coordinates. As a consequence, going back to Cartesian coordinates, we obtain
\[
\int d^4r \, \text{Re}(\tilde{\rho}(\mathbf{r}) R(-\theta) |\Psi_{\theta,0}\rangle^2 = \cos(3\theta).
\]

Therefore, the normalization factor \(1/\sqrt{\cos(3\theta)}\) has to be included in the wave function \(\Phi_{\mathbf{r}}(\mathbf{r})\).

### 2.2. Driven helium atom

In the dipole approximation, length gauge and neglecting relativistic effects, the Hamiltonian for the helium atom in presence of an external electromagnetic field reads

\[
H = H_0 + F(x_1 + x_2) \cos(\omega t),
\]

where \(H_0\) is the unperturbed Hamiltonian (1) and the time-periodic field is linearly polarized along the \(x\) direction with amplitude \(F\) and frequency \(\omega\).

In our approach to solve the time-dependent Schrödinger equation (TDSE)

\[
i \frac{\partial}{\partial t} |\psi(t)\rangle = H |\psi(t)\rangle,
\]

we use a spectral method combined with Floquet theory \([28, 29]\). The method is based on the solution of the TDSE in the atomic basis \(\{|\varphi_i^f\rangle\}_i\), that is the set composed of eigenstates of the unperturbed Hamiltonian \(H_0|\varphi_i^f\rangle = \epsilon_i^f|\varphi_i^f\rangle\), for a given value of the total angular momentum \(L\). In this basis, and within the framework of Floquet theory, the matrix representation of (15) is given by

\[
A \Phi_i = \epsilon_i \Phi_i, \quad A = h_0 - k \omega 1 + F,
\]

where \(\Phi_i\) is the solution vector in the atomic basis, \(h_0\) is the diagonal matrix containing the eigenvalues of \(H_0\), \(F\) the matrix representation of \(F(x_1 + x_2)\) and \(k\) is the Floquet quantum number which gives the amount of photons exchanged between the atom and the field.

The time evolution of a Floquet eigenstate \(|\Phi_i\rangle\) is governed by the rotated time evolution operator \([25, 26]\)

\[
U(t_2, t_1) = \sum_{i, k, k'} e^{-i\epsilon_i (t_2 - t_1)} e^{ik_1 x_1} e^{-ik_2 x_2} \times R(-\theta) |\Psi^l_{i,0}\rangle \langle \Psi^l_{k,0}| R(\theta),
\]

where \(\Psi^l_{i,0}\) are the Fourier components of \(|\Psi_{\theta,0}\rangle\) at \(t = 0\).

In this way, the dynamics of the probability amplitude product is given by

\[
\langle \mathbf{r}' | \phi_{\theta}(t) \rangle \langle \phi_{\theta}(t) | \mathbf{r}'\rangle = e^{2i(\text{Im} \, \epsilon_{i,0})t} \sum_{k, k'} e^{-i(k - k') \omega t} \times \{ \langle \mathbf{r}' | R(-\theta) |\Psi^l_{k,0}\rangle \langle \mathbf{r}' | R(-\theta) |\Psi^l_{i,0}\rangle \\
+ \langle \mathbf{r} | R(-\theta) |\Psi^l_{i,0}\rangle \langle \mathbf{r} | R(-\theta) |\Psi^l_{k,0}\rangle^* \},
\]

### 2.3. Unperturbed frozen planet states

The classical frozen planet configuration (FPC) is an asymmetric one-dimensional configuration where both electrons are located on the same side of the nucleus. In this dynamically stable configuration \([30–32]\), the inner electron precesses on highly eccentric ellipses and the outer electron remains nearly equilibrium distance of the adiabatic potential obtained averaging the fast oscillations of the inner electron.

The classical two-electron dynamics restricted to the collinear frozen planet configuration is regular. That can be observed in the phase space configuration presented in figure 1 (right), which is visualized within a Poincaré surface of section obtained by plotting the position \(x_1\) and the momentum \(p_y\) of the outer electron every time the inner electron reaches the nucleus. The numerical computation of the classical dynamics is achieved by the previous regularization of the equations of motion by Kustaanheimo-Stiefel transformations \([33, 34]\).

Starting from the third series \((N = 3)\) of the helium spectrum, the regular phase space of the FPC supports frozen planet states. These are organized in series converging to single ionization thresholds. We denote by \(\mathcal{F}_N^{\text{FP}}\) the FPS occupying the \(n_F\) position in the series converging to the \(N\)th ionization threshold.

To identify the FPS on the helium spectrum we take into account that these states have long lifetime compared to other resonances in the same energy regime. In addition, due to their localization properties along the FPC, the expectation value of the cosine of the angle \(\theta_{12}\), between the two electrons is close to unity \((\cos \theta_{12} \approx 1)\). We verify these localization properties in phase space with the help of Husimi distributions (see \([22]\) for technical details), for instance, figure 1 shows the phase space projections of the ground (middle) and first excited (right) FPS below the \(N = 4\) single ionization threshold (energies and decay rates for those states are identified in table A1). These quantum states are clearly localized along the periodic orbits of the frozen planet configuration in figure 1 (left).
2.4. Driven frozen planet states

In the presence of an external time-periodic electromagnetic field, the dynamics of the collinear FPC takes place in a five-dimensional phase space described by the positions and momenta of the electrons and by the phase \( \omega t \) of the driving field. For near resonant driving \( \omega \approx \omega_1 \) of amplitude \( F < F_1 \) (where \( \omega_1 \) is the frequency of small oscillations of the outer electron around the equilibrium position and \( F_1 \) is the minimum static field necessary to ionize the FPC), the frozen planet dynamics is not affected in a sensitive way and the time scale separation between the fast Kepler oscillations of the inner electron and the slow motion of the outer electron makes possible to map the phase space structure onto a two-dimensional surface by a two-step Poincaré section method [19, 35].

In figure 2 is depicted the two-step Poincaré surface of section obtained for field parameters \( F = 2 \times 10^{-5} \) a.u. and \( \omega = 0.0036 \) a.u., and field phase \( \omega t = 0 \) (left), \( \omega t = \pi/2 \) (center) and \( \omega t = \pi \) (right). The intrinsic island remains basically unaffected by the field during the time evolution, while the resonance island oscillates around the intrinsic island with the same field frequency.

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In figure 2 is depicted the two-step Poincaré surface of section obtained for field amplitude \( F = 2 \times 10^{-5} \) a.u. and frequency \( \omega = 0.0036 \) a.u., for three different field phases \( \omega t \). Under the action of the external electromagnetic field, the classical phase space separates into two regular regions: the intrinsic island (centred at 30 a.u.) and the resonance island which oscillates around the intrinsic island with the field frequency.

Theoretical studies [19–22] suggest that under near-resonantly periodic driving frozen planet states might transform into two-electron nondispersive wave packets, which propagate along the frozen planet trajectory without dispersion.

The solution of the time-dependent Schrödinger equation (15) for the description of such highly excited driven states is a non-trivial task [36]. Previous large scale computations have been unable to completely characterize such objects [22, 37].

We have developed an efficient approach to study the dynamics of doubly excited states of helium under electromagnetic driving. The method, briefly described in section 2.4, has been used in [38] to characterize NDWP in helium. There, we have been found that the most important features of the nondispersive wave packets are a consequence of the one-photon resonant coupling between two frozen planet states of different angular momentum. In section 3.2, we shall use this result to identify NDWP in the Floquet spectrum of driven helium, below the \( N = 3 \) and 4 ionization thresholds.
2.5. Entanglement measure
For a pure state \(|\Phi\rangle\) of two identical fermions, the Schmidt decomposition in an orthonormal basis of one-particle states \(|i\rangle\) is given by [39, 40]

\[
|\Phi\rangle = \sum_i \sqrt{\lambda_i / 2} (|2i\rangle |2i + 1\rangle - |2i + 1\rangle |2i\rangle),
\]

(19)

where the Schmidt coefficients \(\lambda_i\) satisfy \(0 \leq \lambda_i \leq 1\) and \(\sum_i \lambda_i = 1\). If the state \(|\Phi\rangle\) can be expressed as a single Slater determinant (only one Schmidt coefficient) the state has no entanglement [40–42]. In such a way, the decomposition (19) leads to a measure of the amount of entanglement exhibited by the two-fermion state, namely [40, 41]

\[
\mathcal{E}(|\Phi\rangle) = 1 - \sum_i \lambda_i^2 = 1 - 2 \text{Tr}(\rho^2),
\]

(20)

where \(\rho = \text{Tr}_2(|\Phi\rangle\langle\Phi|)\) is the reduced density matrix (obtained by tracing the two-particle density matrix over one of the two particles).

The state of the two-electron system is described by wave functions of the form

\[
\Phi = \phi(\vec{r}_1, \vec{r}_2) \chi(\sigma_1, \sigma_2),
\]

(21)

where \(\phi(\vec{r}_1, \vec{r}_2)\) and \(\chi(\sigma_1, \sigma_2)\) correspond to the coordinate and spin wave functions, respectively. The corresponding density matrix is expressed as the product \(\rho = \rho^{(\text{coord.})} \otimes \rho^{(\text{spin})}\) and the entanglement measure (20) transforms into

\[
\mathcal{E}(|\Phi\rangle) = 1 - 2 \text{Tr}[\rho^{(\text{coord.})}_1^2 \text{Tr}[\rho^{(\text{spin.})}_1]],
\]

(22)

In this work, we focus on singlet states with anti-parallel spins for which \(\text{Tr}[\rho^{(\text{spin.})}_1] = 1/2\). This lead to the measure

\[
\mathcal{E}(|\Phi\rangle) = 1 - \text{Tr}[\rho^{(\text{coord.})}_1],
\]

(23)

which coincide with the spatial linear entropy. To calculate the entanglement measure (23), we need the computation of the quantity

\[
\text{Tr}[\rho^{(\text{coord.})}_1] = \int \rho^{(\text{coord.})}_1 d\vec{r}_1 d\vec{r}_2,
\]

(24)

where

\[
\rho^{(\text{coord.})}_1 = \int \phi(\vec{r}_1', \vec{r}_2) \phi^*(\vec{r}_1, \vec{r}_2) d\vec{r}_1' d\vec{r}_2.
\]

(25)

The expressions for \(\phi(\vec{r}')\phi^*(\vec{r})\) are obtained from (10) for unperturbed states and from (18) for driven FPS.

For planar helium, the expression (24) corresponds to a 8-dimensional definite integral. We perform this calculation using the VEGAS algorithm included in the Cuba library [43, 44]. VEGAS is widely used for Monte Carlo multidimensional numerical integration and is primarily based on importance sampling, but it also does some stratified sampling as a variance-reduction technique. The algorithm iteratively builds up a piecewise constant weight function, represented on a rectangular grid, which is refined after each iteration. Further details can be found in [45].

3. Results and discussion

3.1. Entanglement in bound and doubly excited states
We calculate the amount of entanglement for the lowest bound and doubly excited \(^1\text{S}\) and \(^1\text{P}\) states below the \(N = 2, 3\) and 4 ionization thresholds. Going beyond the 4th ionization threshold is a difficult task due to the huge number of integrand evaluations needed in (24) to obtain a converged Monte Carlo integration: the region in configuration space where the probability density is non-negligible scales in each direction as \(N^2\) [22]. Therefore, the integration volume in the 8th dimensional integral (24) scales as \(N^{16}\). This is approximately the scaling factor of the number of integrand evaluations and also of the computation time. For instance, while the computation time for states below the 4th ionization threshold is three days, the expected one for states below the 5th ionization threshold is 35 times large. This also might explain why available full three-dimensional calculations are restricted to states below the second ionization threshold.

In table 1, we present the energies and the amount of entanglement for singlet bound states of planar helium. For bound \(^1\text{S}\) states the entanglement increase with energy, whereas for bound \(^1\text{P}\) states, the entanglement increase

\[3\text{ The source code is available from http://feynarts.de/cuba.}\]
decrease with energy. These results are consistent with the entanglement behaviour observed in previous works in three-dimensional helium for low lying excited states \cite{12, 15}.

In the case of DES, it can be observed that the amount of entanglement have different behaviour according to their value of $\cos 12 \theta_2$, which, as we mentioned in section 2.3, is an important quantity to identify the frozen planet states which lead to the formation of NDWP. In figure 3 (left panels) we present the amount of entanglement as a function of the energy for doubly excited $^1S$ states. The results are organized in series that can

| $N, n$ | $^{1S}$ | $^{1P}$ |
|-------|--------|--------|
| 1, 1  | 11.899 822 343 | 0.010 8 |
| 1, 2  | 8.250 463 875 | 0.696 7 |
| 1, 3  | 8.085 842 793 | 0.750 1 |
| 1, 4  | 8.042 911 011 | 0.751 0 |
| 1, 5  | 8.025 668 310 | 0.752 4 |
| 2, 1  | 8.211 542 09 | 0.999 99 |
| 2, 2  | 8.077 637 33 | 0.938 80 |
| 2, 3  | 8.039 947 88 | 0.731 43 |
| 2, 5  | 8.024 280 94 | 0.752 6 |

**Table 1.** Energies and entanglement of the lowest bound $^1S$ and $^1P$ states of planar helium.

![Figure 3](image-url) Entanglement (left) and $\langle \cos \theta_{12} \rangle$ (right) against energy of the lowest $^1S$ doubly excited states below the $N$th single ionization threshold (indicated by vertical dashed lines). The results are organized in series according to their value of $\langle \cos \theta_{12} \rangle$.

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be related to the value of \( \langle \cos \theta_{12} \rangle \) as we observe in the right panels of figure 3, where we show the expectation values of \( \cos \theta_{12} \) as a function of the energy. Similar behaviour is presented for doubly excited \( \text{P}^1 \) states in figure 4. The converged values of the entanglement measure are presented in the appendix.

In our results for DES below the \( N = 2 \) ionization threshold, the amount of entanglement in the different series increases to reach a maximum value and then decreases, with exception of the \( \text{P}^1 \) states with
In the atomic basis containing only the states $|a\rangle \equiv 1S^2F_a^N$ and $|b\rangle \equiv 1P^2F_b^N$. In that basis, the matrix representation of the Floquet Hamiltonian is given by

$$A = \begin{pmatrix} E_a + \omega & F_{ab} \\ F_{ba} & E_b \end{pmatrix},$$

where $E_{ab} = \langle a|F|x_b \rangle (x_b + x_a)/2|b\rangle$, and $E_a$ is the complex energy of the resonance state $|a\rangle$.

In the Floquet spectrum obtained after diagonalization of (26), we identify nondispersive wave packets below the $N = 3$ and 4 ionization thresholds. For $N = 3$ we use the field parameters $F = 4 \times 10^{-5}$ a.u. and $\omega = 0.006$ 6 a.u. The wave packet below the $N = 3$ ionization threshold has energy $E = -0.342 610 1$ a.u. and decay rate $\Gamma = 8 \times 10^{-7}$ a.u. For the case of $N = 4$ the field parameters are $F = 2 \times 10^{-5}$ a.u. and $\omega = 0.003 6$ a.u., and the energy and decay rate wave of the packet are $E = -0.175 769 8$ a.u. and $\Gamma = 4.5 \times 10^{-6}$ a.u., respectively.
Figure 5 displays the phase space projection of the $N = 4$ singlet wave packet, which can be compared with the classical phase space structure presented in figure 2, obtained for the same driving field parameters. Clearly, the wave packet motion in figure 5 is associated with the dynamics of the resonance island in the classical phase space.

Figure 6 shows the amount of entanglement calculated as a function of the driving field phase for the the two wave packets. For comparison, we also show the amount of entanglement for the FPS involved in the formation of the NDWP and the time-average entanglement $\bar{E}$ over one period $T$

$$\bar{E} = \frac{1}{T} \int_0^T E(t) \, dt. \quad (27)$$

For the wave packet below the third ionization threshold (figure 6 (top)) the time-average entanglement $\bar{E}$ was approximately the mean value between the amount of entanglement of the $^1S_F^2$ and $^1P_F^2$ frozen planet states, while for the wave packet below the fourth ionization threshold (figure 6 (bottom)), the time-average entanglement was greater than the values for the initial FPS. In both cases $N = 3$ and $N = 4$, we observe that the maximum values for the wave packet entanglement were for the driving field phases $\omega t = \pi/2$ and $\omega t = 3\pi/2$.

### 4. Summary and conclusions

In this work, we have calculated the amount of entanglement of bound and doubly excited states below the $N = 2, 3$ and 4 ionization thresholds for planar helium. Additionally, we computed the entanglement of nondispersive two-electron wave packets produced by frozen planet states driven by an external periodic field.

We found that for bound $^1S$ states the entanglement increase with energy while for bound $^1P$ states the entanglement decrease with energy. For DES below the $N = 2$ ionization threshold, the entanglement values are organized in series where the entanglement reaches a maximum before decreasing. These results are consistent with that observed in three-dimensional calculations [15]. In both cases $N = 3$ and $N = 4$, the entanglement values for FPS are higher than for the other series of states (above 0.92 for $N = 4$ and 0.89 for $N = 3$) and we also found that the amount of entanglement of $^1P$ FPS is greater than for $^1S$ FPS for each series. We expect that this behaviour could be verified on three-dimensional computations. On the other hand, it would be interesting to extend the calculations to highly doubly excited states and higher angular momenta, and for those states verify the general trend of entanglement to increase with the strength of the inter-particle interaction and its non-vanishing value in the limit of zero interaction [51].

In the case of driven FPS, we found that the time-average entanglement for NDWP below the $N = 4$ ionization threshold is greater than the entanglement of the unperturbed FPS involved in its formation. Although only fixed driving field parameters were used here, the NDWP produced by driven FPS maintain their behaviour under driving field amplitude and frequency variations [38]. Thus, investigation of the effect of the field parameters variation on the amount of entanglement in NDWP is feasible.

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### Appendix. Entanglement data for DES

This appendix contains the entanglement values for the doubly excited $^1S$ and $^1P$ states below the $N = 2, 3$ and 4 ionization thresholds, discussed in section 3.1.

In tables A1 and A2 we present the energies, decay rates and the amount of entanglement for doubly excited $^1S$ and $^1P$ states, respectively. Additionally, we include the expectation value of $\cos \theta_{12}$. In the second column of each table we identify the lowest FPS of the series converging to the third and fourth ionization thresholds.
Table A1. Energies and entanglement of the lowest $^1S$ doubly excited states below the $N$th single ionization threshold. Decay rates and the expectation value of $\cos \theta_{12}$ are also shown.

| $N = 2$ | $-\mathcal{E}$ [a.u.] | $\Gamma/2$ [a.u.] | $\langle \cos \theta_{12} \rangle$ | $\mathcal{E}$ |
|---------|----------------|-----------------|------------------|------|
| 1.411 496 33 | 0.001 241 73 | -0.641 | 0.528 | 1 |
| 1.027 047 55 | 0.000 251 80 | 0.165 | 0.657 | 0 |
| 1.016 821 16 | 0.000 106 49 | -0.305 | 0.795 | 5 |
| 0.947 988 02 | 0.000 103 36 | -0.305 | 0.610 | 4 |
| 0.945 091 77 | 0.000 003 69 | 0.278 | 0.791 | 0 |
| 0.921 743 53 | 0.000 044 79 | -0.398 | 0.651 | 4 |
| 0.920 365 12 | 0.000 000 49 | 0.387 | 0.828 | 1 |
| 0.909 741 13 | 0.000 022 96 | -0.429 | 0.633 | 0 |
| 0.908 994 46 | 0.000 000 12 | 0.423 | 0.816 | 0 |

$\mathcal{F}^1_1$:
| 0.516 872 10 | 0.001 165 79 | -0.757 | 0.625 | |
| 0.371 886 03 | 0.000 684 06 | -0.014 | 0.843 | 0 |
| 0.362 061 79 | 0.000 219 92 | -0.782 | 0.836 | |

$\mathcal{F}^1_2$:
| 0.354 907 55 | 0.000 037 37 | 0.672 | 0.895 | 0 |
| 0.349 336 28 | 0.000 311 35 | 0.046 | 0.863 | 2 |
| 0.345 721 87 | 0.000 106 60 | -0.784 | 0.854 | |

$\mathcal{F}^2_2$:
| 0.342 496 48 | 0.000 048 48 | 0.676 | 0.904 | |
| 0.338 947 12 | 0.000 166 03 | 0.071 | 0.866 | |
| 0.337 233 25 | 0.000 058 60 | -0.785 | 0.865 | |

$\mathcal{F}^2_3$:
| 0.335 495 10 | 0.000 007 07 | 0.680 | 0.897 | |
| 0.333 257 83 | 0.000 098 48 | 0.083 | 0.864 | |
| 0.332 312 68 | 0.000 035 37 | -0.785 | 0.859 | |

$\mathcal{F}^3_3$:
| 0.265 531 28 | 0.000 774 57 | -0.820 | 0.680 | 1 |
| 0.214 973 81 | 0.000 509 11 | 0.119 | 0.700 | 96 |
| 0.214 716 02 | 0.000 436 21 | -0.821 | 0.842 | 5 |
| 0.202 667 79 | 0.001 395 54 | -0.267 | 0.802 | 3 |
| 0.194 378 58 | 0.000 222 19 | -0.839 | 0.863 | 5 |
| 0.188 805 39 | 0.000 108 16 | 0.206 | 0.782 | 13 |
| 0.187 411 99 | 0.000 791 48 | -0.266 | 0.791 | 3 |
| 0.183 759 94 | 0.000 116 31 | -0.843 | 0.876 | |
| 0.180 560 51 | 0.000 000 88 | 0.788 | 0.926 | 9 |
| 0.179 914 71 | 0.000 034 17 | 0.198 | 0.792 | |
| 0.179 550 43 | 0.000 480 43 | -0.212 | 0.795 | |
| 0.177 663 08 | 0.000 065 86 | -0.845 | 0.881 | |

Table A2. Energies and entanglement of the lowest $^1P$ doubly excited states below the $N$th single ionization threshold. Decay rates and the expectation value of $\cos \theta_{12}$ are also shown.

| $N = 2$ | $-\mathcal{E}$ [a.u.] | $\Gamma/2$ [a.u.] | $\langle \cos \theta_{12} \rangle$ | $\mathcal{E}$ |
|---------|----------------|-----------------|------------------|------|
| 1,153 941 04 | 0.000 128 21 | 0.087 | 0.587 | 60 |
| 1,031 093 30 | 0.000 000 11 | -0.599 | 0.818 | 05 |
| 0.966 997 08 | 0.000 019 51 | 0.075 | 0.796 | 0 |
| 0.953 526 23 | 0.000 000 03 | 0.502 | 0.911 | 8 |
| 0.949 895 59 | 0.000 000 03 | -0.614 | 0.853 | 9 |
| 0.928 609 96 | 0.000 007 46 | 0.079 | 0.792 | 3 |
| 0.923 888 21 | 0.000 000 01 | 0.527 | 0.906 | 7 |
| 0.922 496 28 | 0.000 000 01 | -0.620 | 0.884 | 6 |
| 0.912 996 73 | 0.000 003 61 | 0.080 | 0.780 | 8 |

$\mathcal{F}^2_1$:
| 0.405 019 34 | 0.000 007 35 | -0.759 | 0.796 | 8 |
| 0.384 454 91 | 0.002 026 90 | -0.193 | 0.816 | 3 |
| 0.381 575 84 | 0.000 334 31 | 0.103 | 0.858 | 9 |
| 0.378 800 09 | 0.000 008 63 | 0.012 | 0.866 | 1 |
| 0.363 904 50 | 0.000 004 31 | -0.768 | 0.831 | 0 |
| 0.354 875 71 | 0.000 955 57 | -0.312 | 0.861 | 9 |
Table A2. (Continued.)

| \(N\) | \(-\mathcal{E}\) [a.u.] | \(\Gamma/2\) [a.u.] | \(\langle \cos(\theta)\rangle\) | \(\mathcal{E}\) |
|-------|-----------------|----------------|----------------|-------------|
| \(N = 4\) | | | | |
| 0.352 224 93 | 0.000 051 40 | 0.363 | 0.843 3 |
| 0.351 767 14 | 0.000 015 33 | 0.016 | 0.869 6 |
| \(\mathcal{F}_1\) | 0.348 950 78 | 0.000 009 09 | 0.616 | 0.911 4 |
| \(\mathcal{F}_1\) | 0.338 858 83 | 0.000 005 05 | 0.608 | 0.905 7 |
| 0.337 615 38 | 0.000 001 42 | -0.775 | 0.824 |
| 0.181 531 26 | 0.000 298 62 | -0.531 | 0.892 |
| \(\mathcal{F}_1\) | 0.179 248 39 | 0.000 013 53 | 0.693 | 0.929 2 |
| \(\mathcal{F}_1\) | 0.177 914 28 | 0.000 004 14 | -0.838 | 0.836 |
| \(\mathcal{F}_1\) | 0.177 295 39 | 0.000 239 32 | 0.056 | 0.906 |

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