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Tunneling through Coulombic barriers: quantum control of nuclear fusion

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A general coherent control scheme for speeding up quantum tunneling of proton transfer through Coulombic barriers is analysed. The quantum control scenario is based on repetitive electron impact ionization pulses that affect the ensuing interference phenomena responsible for quantum dynamics and force the proton to tunnel into classically forbidden regions of configuration space. The scheme is demonstrated for the simplest model of nuclear fusion, hinting at the possible enhancement of reactive scattering based on low energy collisions.

Keywords: quantum dynamics; proton tunneling; coherent control; nuclear fusion; bang-bang

1. Introduction

Control of self-sustained nuclear fusion reactions (e.g. the reactions that generate solar energy) is an outstanding challenge of the 21st century [1]. Nuclear reactions of heavy hydrogen isotopes (D^+ and T^+),

$$D^+ + D^+ \rightarrow {}^3He^{2+} + n,$$
$$D^+ + T^+ \rightarrow {}^4He^{2+} + n,$$

produce He, neutrons n, and an enormous amount of energy ($U_0 = 3.27$ and 17.59 MeV, for the D–D and D–T reactions given above, respectively). Therefore, they are particularly attractive for energy applications. However, in order to fuse, the positively charged nuclei (e.g. d D^+ and T^+) have to overcome MeV Coulombic barriers (V_b) [2] (Figure 1). Thus, the challenge is to reach a controlled reaction condition where the energy necessary to overcome the Coulombic barrier is less than the energy released by fusion.

Most current research efforts are focused on methods to generate the thermonuclear regime, with high temperature and compression achieved by high magnetic fields, or under laser induced implosion [2–4]. Traditional plasma simulations are usually based on classical models. However, there is the non-trivial question as whether quantum effects could influence the reaction cross-sections, due to quantum statistics, tunneling, or even quantum coherences, under drastic *confinement* conditions (particularly for laser induced inertial confinement) [5]. While a full quantum treatment of high-density plasmas represents an enormous computational challenge, studies of model systems [6,7] can already provide insights into fundamental aspects that remain poorly understood. In this work, we focus on the analysis of quantum tunneling through Coulombic barriers and we explore the feasibility of quantum control leading to low energy paths for nuclear fusion.

The main difficulty hindering the pursuit of fusion in the non-thermonuclear regime, is the extremely small transmission probability for low energies collisions, as determined by the Coulombic barriers [8]. The transmission probability gives the fusion rate as determined by the collision cross-section and the tunneling probability. A good estimate of this probability is given by the Gamow formula [2,9,10]:

$$\sigma(E) = \frac{A}{E}\exp\left(-\frac{B}{E^{1/2}}\right), \quad (1)$$

where E is the total collision energy of the approaching nuclei (Figure 1) in their centre-of-mass frame, and the constants A and B, are defined by the size and nature of the colliding nuclei. At low energies, Equation (1) predicts very small cross sections. For example, the fusion cross sections $\sigma(E)$ for the reactions D–D and D–T, given above, are 0.11 and 5 barns (1 barn = 10^{-24} cm^2), respectively, at centre-of-mass energy $E = 100$ keV. This is due to the small size of the nuclei, making collisions rare events unless the nuclei move at very high velocities. Increasing the density would obviously increases the collision rates. However, even for frequent low-energy collisions reactive events are still forbidden by the insurmountable Coulombic barriers (of a few MeV), with negligible tunneling probabilities [8].

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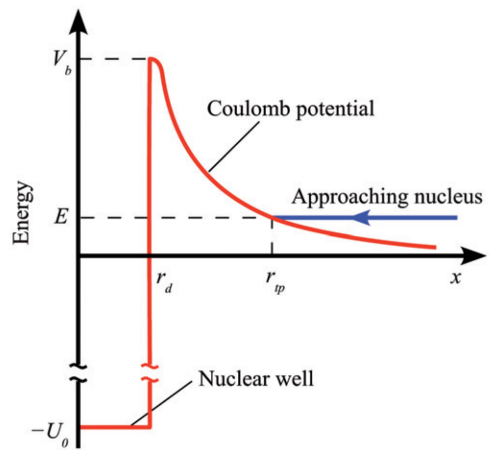

Figure 1. Potential energy surface, as a function of the interdeuteron distance, describing the nuclear fusion reaction $2D^+ \rightarrow {}^3He^{2+} + n$.

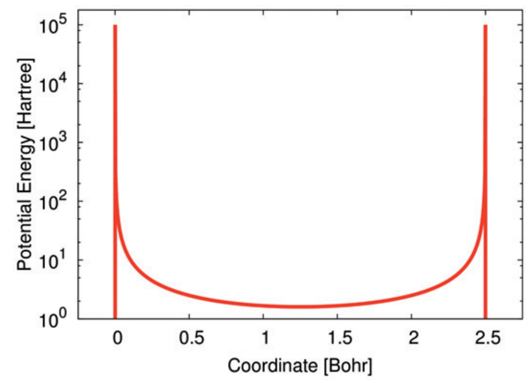

Figure 2. Potential energy surface of D^+ ion in a one-dimensional box, interacting with another D^+ at the origin and periodic boundary conditions (or two D^+ ions in a 1-dimensional ring).

High transmission is achieved with over-the-barrier high-energy collisions as in the thermonuclear regime [11–14]. However, reactive under-the-barrier collisions have been much less investigated. Here, we explore whether tunneling could be enhanced by the perturbational influence of external fields. The proposed method is based on sequences of low-energy electron impact ionization pulses that affect quantum interferences amongst characteristic reactive channels. The method builds upon previous work on quantum control based on optical pulses [15–18], inspired by coherent control techniques [19], closely related to bang-bang dynamical decoupling methods [16, 20]. The essential ingredient of these quantum control techniques is the application of unitary perturbational pulses that affect the ensuing interferences and elicit the desired dynamical behavior.

2. Methods and model system

Figure 2 shows the model potential energy surface (PES) for a D^+ in a one-dimensional box with periodic boundary conditions, interacting with another D^+ at the origin. The size of the box $x_0 = 2.5$ *a.u.* is defined by the plasma density, mimicking a D^+ interacting with its nearest neighbours in a high-density plasma.

This one-dimensional model also represents the interaction of two D^+ ions trapped in a ring, as described by the sum of repulsive Coulombic potentials:

$$V = \begin{cases} \dfrac{1}{|x|} + \dfrac{1}{|x - x_0|}, & \text{when } |x| \text{ or } |x - x_0| > r_d \\ -U_0 + iU_a(x), & \text{otherwise.} \end{cases} \tag{2}$$

The optical potential $iU_a(x)$ absorbs the outgoing flux, leaking into the other side of the barrier with $|x| < r_d$, or $|x - x_0| < r_d$, mimicking the outgoing flux leaking into the continuum of translational states $|k\rangle$ of helium ions and neutrons generated by reactive collisions. Therefore, the decay of the wavefunction amplitude quantifies the amount of fusion.

Here, $r_d = 1.44 \cdot 10^{-13}\,(A_1^{1/3} + A_2^{1/3})$ cm is defined by the sum of the radii of the two nuclei with mass numbers A_1 and A_2 (Figure 1).

The initial state $|\psi_0\rangle$, describing the two D^+ ions in the ring, is defined as generated by impulsive ionization of the D_2 molecule, according to the vibrational ground state of D_2. The ensuing time-evolution is simulated by using the standard Split Operator Fourier Transform (SOFT) method [22].

Each perturbational pulse simulates an electron scattering event [23,24] that transiently transfers the vibrational component $|s\rangle$ to the D_2^+ surface, while the electron approaches the D_2^{2+} pair, and then regenerates the population in the D_2^{2+} state when the electron continues its outbound trajectory and departs from the system (Figure 3). The duration of the electron scattering process is chosen to produce a π phase-shift along the $|s\rangle$ vibrational component of the time-evolving wavepacket. With such pulse duration, the resulting perturbational effect of a pulse can be represented by the unitary operator [17],

$$U^{2\pi} = 1 - 2|s\rangle\langle s|, \tag{3}$$

called a 2π pulse in the optics community, or a 180-pulsein the context of spin-echo NMR.

The net perturbational effect of a train of unitary pulses $U^{2\pi} = 1 - 2|s\rangle\langle s|$ has been recently analyzed by using a perturbation treatment [18], analogous to the

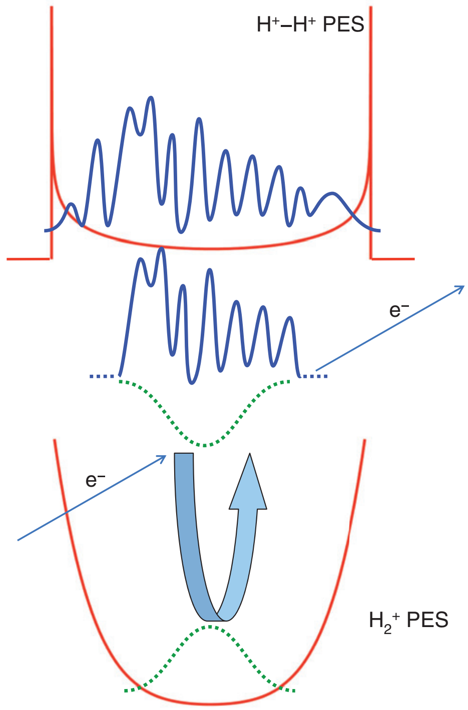

Figure 3. Electron-impact ionization events couple the D_2^{2+} and D_2^+ states affecting the interference phenomena and ultimately the tunneling dynamics across the Coulombic barrier.

study reported for other control schemes [21]. The treatment is based on the general Hamiltonian,

$$H = \omega_s|s\rangle\langle s| + \sum\nolimits_k \omega_k|k\rangle\langle k| + \sum\nolimits_k V_{ks}|k\rangle\langle s| + V_{sk}|s\rangle\langle k| \tag{4}$$

where the matrix elements V_{ks} define the couplings between the bound state $|s\rangle$ and the continuum. Such treatment gives the early time-dependent population of $|s\rangle$ and its decay rate Γ_{pulse} under repetitive pulsing:

$$\begin{aligned} P_s(t) &= \left|\langle s|\left(\hat{U}^{2\pi}e^{-i\hat{H}\Delta t}\hat{U}^{2\pi}e^{-i\hat{H}\Delta t}\right)^n|s\rangle\right|^2 \\ &= (1-\Gamma_{\text{pulse}}t) \approx e^{-\Gamma_{\text{mod}}t} \\ \Gamma_{\text{pulse}} &= \sum_k |V_{ks}|^2\tan^2\left(\{\omega_k-\omega_s\}\frac{\Delta t}{2}\right)\frac{\sin^2(\omega_k-\omega_s)\frac{2n\Delta t}{2}}{\left(\frac{\omega_k-\omega_s}{2}\right)^2} \end{aligned} \tag{5}$$

with $t = n\,2\Delta t$, and Δt the time-interval between pulses. In contrast, in the absence of pulses, the spontaneous decay rate is

$$\Gamma_{\text{no-pulse}} = \sum_k |V_{ks}|^2\frac{\sin^2(\omega_k-\omega_s)\frac{2n\Delta t}{2}}{\left(\frac{\omega_k-\omega_s}{2}\right)^2}. \tag{6}$$

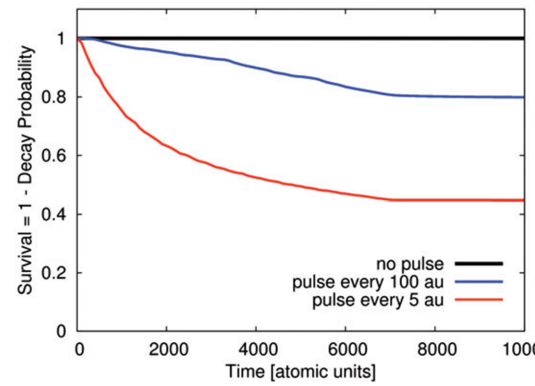

Figure 4. Time-dependent survival probability showing decay of wavepacket norm with pulses. The black line shows that without any pulse decay is negligible. Decay increases with pulsing shown using red and blue lines.

Comparing Equations (5) and (6), it is clear that the decay with pulses is faster than spontaneous decay when $\tan^2(\omega_k-\omega_s)\frac{\Delta t}{2} > 1$. Therefore, we explore pulsing schemes that satisfy such condition.

3. Results

Dynamics simulations are performed in the time-dependent picture by implementing the split operator Fourier transform method, as previously reported [25,26], based on a grid- representation of equally spaced delta functions in coordinate space. Figure 4 compares the time-dependent survival probability,

$$P(t) = \int_{r_d}^{x_0-r_d} \mathrm{d}x\langle x \mid \Psi_t\rangle\langle\Psi_t \mid x\rangle, \tag{7}$$

for the unperturbed system (no pulse) to the evolution affected by pulses (pulse every 5 or 100 a.u.). These results show that although decay is negligible in the absence of pulses, it becomes quite significant with frequent perturbational pulses coupling the bound states to the continuum. The slope of $P(t)$ at the early time ($t \to 0$) gives the tunneling rate. The asymptotic value, at long time ($t \to \infty$), gives the product yield $R(t) = 1 - P(t)$. These results indicate that tunneling becomes faster and more significant with frequent pulses (see population decay of $>20\%$ when pulsing every 100 a.u. and increasing to $>50\%$ with an increased pulsing rate in consonance with Equation (5)).

Figure 5 compares the evolution of the probability amplitude $\rho_t(x) = \Psi_t(x)^*\Psi_t(x)$, obtained for the evolution of the system with (and without) perturbational pulses. In the absence of pulses, the profile of the coherent wavepacket remains localized, with low frequency modulations superimposed to the initial

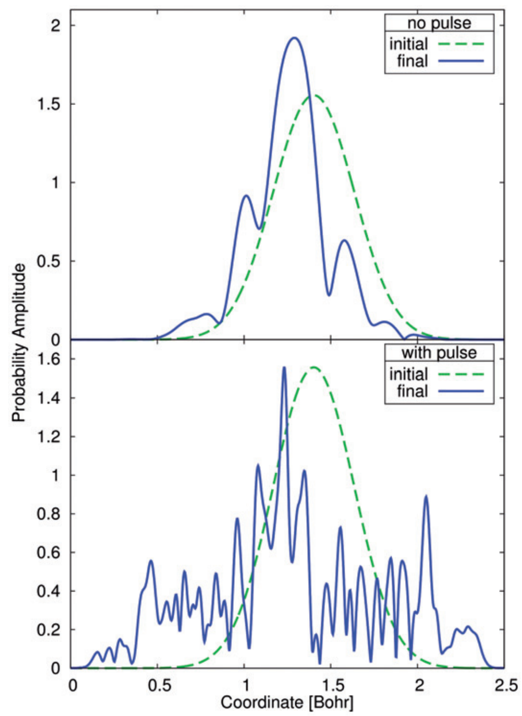

Figure 5. Squared amplitudes of initial (green dashed) and time-evolved (blue solid) wavepackets, propagated unperturbed (top) or under the influence of a sequences of perturbational pulses (bottom) as described in the text.

Gaussian profile. In contrast, with perturbational pulses, the wavepacket acquires a highly oscillatory amplitude profile. The sequence of π phase-shifts along the $|s\rangle$ component cause destructive interference among various bound wavepacket components as well as constructive interference inside the Coulombic barrier and beyond. The net effect of the couplings is to redistribute population among energy levels, without significantly affecting the total energy of the system (Figure 6). The resulting perturbed wavefunction thus consists of a superposition of eigenstates, including population of the continuum (absorbed by the optical potential) as well as components of higher energy states responsible for the oscillations inside the Coulombic barrier. These components are formed at the expense of depletion of lower energy states.

This is supported by the energetic and population analysis, shown in Figure 6, for the initial and time-evolved states, as decomposed in the basis of particle-in-the-box states (box-size x_0) which are similar to the eigenstates of the model potential well (note that Figure 2 is drawn at a logarithmic scale). The state distribution shows that both the initial and time-evolved state at $t = 2000$ a.u., while the population is still decaying, can be represented with low-energy

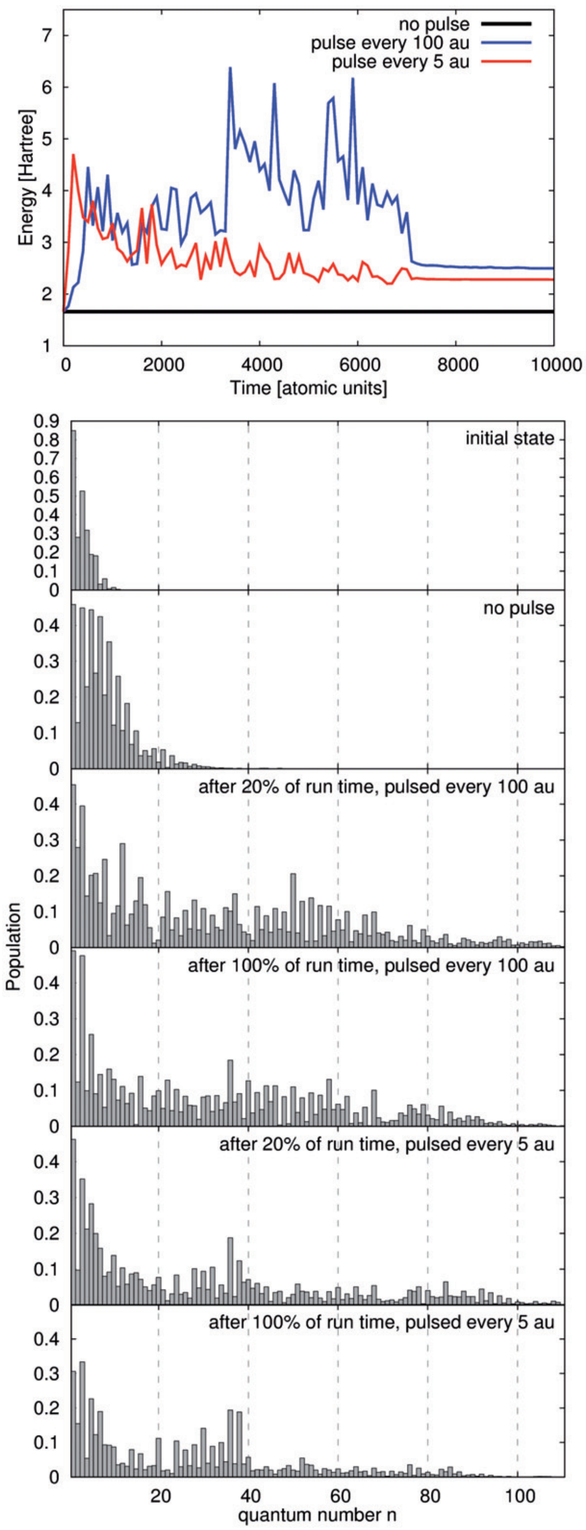

Figure 6. Top: Energy of the survival population obtained with no pulses (black), or exposed to pulses every 100 a.u. (red), or every 5 a.u. (blue). Bottom: Population of particle-in-the-box bound states with $n = 1 - 120$, distributing the initial ($t = 0$) and the time-evolved state ($t = 242$ fs, 10^4 a.u.), obtained without perturbational pulses, or pulsing every 100 or 5 a.u. Note that the population remains distributed among low energy ($E(n = 100) = 4.3$ a.u. $\ll V_{b}. = 10^5$ a.u.).

states ($n < 100$, $E < 4.3$ a.u.). The decay of the population in the presence of pulses demonstrates that tunneling into the continuum of fusion states can proceed from these relatively low-lying states. The energetic analysis is based on the computation of the time-dependent expectation value,

$$E(t) = P(t)^{-1} \int_{r_d}^{x_0 - r_d} \Psi_t(x)^* \hat{H} \Psi_t(x)\, \mathrm{d}x \tag{8}$$

providing a quantitative analysis of the average energy of the bound population. Energy fluctuations are observed due to the exchange of energy with the perturbational field. The resulting energy fluctuations are much smaller (<7 Hartree) than the Coulombic energy barrier in the MeV (10^5 Hartree) range, showing reactive scattering based on low-energy collisions.

In summary, we note that the manipulation of quantum coherences by sequences of unitary phase-kick pulse induces significant tunneling without changing much the energy of the system. Observing the predicted quantum control, however, would require sufficiently high collision cross sections (high density, or high temperature) and the survival of quantum coherences during the time scale of reactive scattering event.

4. Conclusions and outlook

The goal of self-sustained fusion in the laboratory still evades current technology in spite of significant efforts, as the huge energetic demands required by thermonuclear experiments prevent break-even conditions. The results reported in this paper predict that D^+ tunneling through MeV Coulombic barriers could be induced by sequences of low-energy electron impact ionization pulses. However, the control scheme is expected to be most effective under conditions that would ensure sufficiently high collision cross-sections and long decoherence times. onsidering the time-scales involved, however, the predicted quantum control should be observed unless the decoherence time is much shorter than 200 fs. It is, therefore, suggested that electron impact ionization pulsing during the final ignition step of inertial confinement [12], under such conditions, could yield efficiency gains necessary to reach break-even conditions in the pursuit of sustainable fusion.

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References

[1] G.M. McCracken and P. Stott, *Fusion: The Energy of the Universe* (Elsevier Academic Press, Burlington, MA, 2005).
[2] G.A. Moses and J.J. Duderstadt, *Inertial Confinement Fusion* (John Wiley & Sons, New York, 1982).
[3] A.H. Boozer, Rev. Mod. Phys. **76**, 1071 (2004).
[4] J.D. Lindl, P. Amendt, R.L. Berger, S.G. Glendinning, S.H. Glenzer, S.W. Haan, R.L. Kauffman, O.L. Landen and L.J. Suter, Phys. Plasmas **11**, 339 (2004).
[5] P.K. Shukla, Nat. Phys. **5**, 92 (2009).
[6] D. Klakow, C. Toepffer and P.G. Reinhard, J. Chem. Phys. **101**, 10766 (1994).
[7] D. Shaikh and P.K. Shukla, Phys. Rev. Lett. **99**, 125002 (2007).
[8] A.B. Balantekin and N. Takigawa, Rev. Mod. Phys. **70**, 77 (1998).
[9] G. Gamow and E. Teller, Phys. Rev. **53**, 608 (1938).
[10] S. Ichimaru and H. Kitamura, Phys. Plasmas **6**, 2649 (1999).
[11] S. Chelkowski, A.D. Bandrauk and P.B. Corkum, Phys. Rev. Lett. **93**, 083602 (2004).
[12] K. Imasaki and D. Li, Laser Particle Beams **26**, 3 (2008).
[13] A.V. Sokolov and M. Zhi, J. Mod. Opt. **51**, 2607 (2004).
[14] G. Kalbermann, Phys. Rev. C (Nucl. Phys.) **77**, 041601 (2008).
[15] L.G.C. Rego, S.G. Abuabara and V.S. Batista, J. Mod. Opt. **53**, 2519 (2006).
[16] L.G.C. Rego, L.F. Santos and V.S. Batista, Annu. Rev. Phys. Chem. **60**, 293 (2009).
[17] L.G.C. Rego, S.G. Abuabara and V.S. Batista, J. Mod. Opt. **54**, 2617 (2007).
[18] R. Saha and V.S. Batista, J. Phys. Chem. B **115**, 5234 (2011).
[19] P.W. Brumer and M. Shapiro, *Principles of the Quantum Control of Molecular Processes* (John Wiley & Sons, New York, 2003).
[20] L. Viola and S. Lloyd, Phys. Rev. A **58**, 2733 (1998).
[21] A.G. Kofman and G. Kurizki, Nature **405**, 546 (2000).
[22] M.D. Feit, J.A. Fleck Jr and A. Steiger, J. Computat. Phys. **47**, 412 (1982).
[23] G. Herzberg, *Molecular Spectra and Molecular Structure I. Spectra of Diatomic Molecules* (Van Nostrand Reinhold, New York, 1950).
[24] M.A. Coplan, J.H. Moore and J.P. Doering, Rev. Mod. Phys. **66**, 985 (1994).
[25] J.C. Burant and V.S. Batista, J. Chem. Phys. **116**, 2748 (2002).
[26] Y.H. Wu and V.S. Batista, J. Chem. Phys. **121**, 1676 (2004).