Resonantly Enhanced Pair Production in a Simple Diatomic Model

François Fillion-Gourdeau,[1,*] Emmanuel Lorin,[2,†] and André D. Bandrauk[3,‡]

[1]Centre de Recherches Mathématiques, Université de Montréal, Montréal, Canada H3T 1J4
[2]School of Mathematics and Statistics, Carleton University, Ottawa, Canada K1S 5B6
[3]Laboratoire de chimie théorique, Faculté des Sciences, Université de Sherbrooke, Sherbrooke Canada J1K 2R1

(Received 28 August 2012; published 2 January 2013)

A new mechanism for the production of electron-positron pairs from the interaction of a laser field and a fully ionized diatomic molecule in the tunneling regime is presented. When the laser field is turned off, the Dirac operator has resonances in both the positive and the negative energy continua while bound states are in the mass gap. When this system is immersed in a strong laser field, the resonances move in the complex energy plane: the negative energy resonances are pushed to higher energies while the bound states are Stark shifted [F. Fillion-Gourdeau *et al.*, J. Phys. A **45**, 215304 (2012)]. It is argued here that there is a pair production enhancement at the crossing of resonances by looking at a simple one-dimensional model: the nuclei are modeled simply by Dirac delta potential wells while the laser field is assumed to be static and of finite spatial extent. The average rate for the number of electron-positron pairs produced is evaluated and the results are compared to the one and zero nucleus cases. It is shown that positrons are produced by the resonantly enhanced pair production mechanism, which is analogous to the resonantly enhanced ionization of molecular physics. This phenomenon could be used to increase the number of pairs produced at low field strength, allowing the study of the Dirac vacuum.

DOI: 10.1103/PhysRevLett.110.013002 PACS numbers: 31.30.J−, 12.20.Ds, 42.50.Hz

There has been a tremendous amount of effort in the last few decades to increase laser intensities and it is now conceivable to reach laser intensities above 10^{23} W/cm^2 [1], such that the corresponding field strength is larger than the Coulomb fields in matter. For slightly lower intensities, this has led to the development of nonperturbative models of ionization such as tunneling ionization in atomic physics [2] and charge resonance enhanced ionization (CREI) in molecular physics [3]. This new regime of superintense laser intensities now available allows the study of new physical effects where relativistic and quantum electrodynamics (QED) corrections start to be important [4]. Among the QED effects, one of the most important phenomena is the long-sought Schwinger mechanism [5], which consists of the decay of the vacuum of a static electric field into electron-positron pairs. In the Dirac interpretation, this can be seen as a tunneling of electrons from the negative energy sea to the positive continuum. This has never been observed experimentally because it requires field strengths on the order of $E_S \sim 10^{18}$ V/m (as compared to atomic Coulomb fields with $E_0 \sim 5 \times 10^{11}$ V/m), which are not available experimentally (this corresponds to a laser intensity of 10^{29} W/cm^2). However, given the new experimental advances and the novel laser technologies, there has been a renewed interest in this process and new ideas have emerged which could allow us to probe the QED vacuum. Therefore, many variations of Schwinger's original idea using different field configurations have been proposed [6–15]. A semiclassical theory of relativistic tunneling ionization has also been considered [16], similar to atomic tunneling ionization.

In this Letter, a new mechanism is proposed to enhance pair production from a laser field interacting with a fully ionized diatomic molecule, which we denote the resonantly enhanced pair production (REPP) process. This mechanism is analogous to the CREI process, which is well known to occur in molecular physics via a Stark shifted molecular Coulomb potential [3]. It proceeds in the following way and is depicted in Fig. 1. First, let us consider the case when the electric field F is zero and look at the spectrum of the Dirac operator for a system having two nuclei. Also, for simplicity, we consider only two bound states: the ground state and the first excited state. If the nuclear charge is not too large ($Z < 137$), the bound states are in the mass gap, in the energy range $[-mc^2, mc^2]$. On the other hand, the negative and positive energy continua incorporate the so-called Ramsauer-Townsend resonances (RTRs) (these are shown as dark regions in Fig. 1), related to the backscattering of waves on the potential wells. This results in a peak-valley structure in the spectral density function in both continua [17]. When the electric field is turned on and the interatomic distance R is varied, the positions of the resonances in the complex energy plane change: the RTRs of the negative energy sea are Stark shifted to higher energies while the RTRs of the positive energy continuum are downshifted towards lower energies [17]. The bound states become resonances (their energies gain an imaginary part and thus become unstable states) and are Stark shifted by $\Delta \sim \pm FR/2$. When a RTR of the negative energy sea crosses a resonance from the bound states or a RTR from the positive energy continuum, the transition from the negative to the positive energy

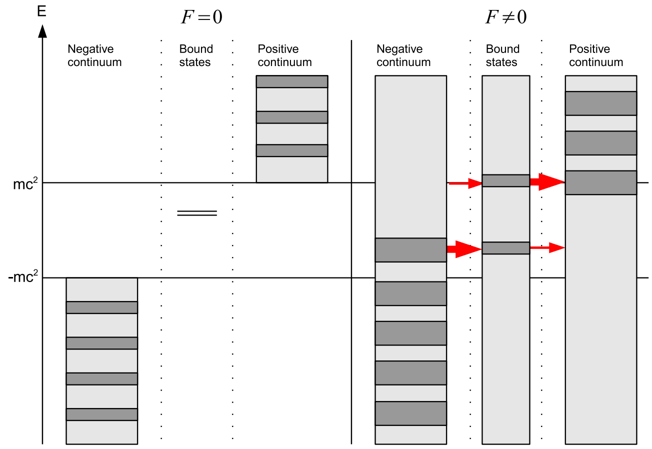

FIG. 1 (color online). Description of the REPP mechanism. The dark gray regions are the positions of resonances (high density of states) while the light gray regions correspond to accessible energies which have a lower density of states.

continuum is enhanced, yielding a higher pair production rate (channel 1). The same mechanism occurs for the excited state: when it crosses a RTR from the positive energy sea, the ionization of the molecule is enhanced, facilitating also the transition from the negative energy sea to the resonance because it reduces the Pauli blocking (if the electron is ionized, the excited state resonance is "free" and can receive a new electron that tunneled from the negative energy state). This is channel 2. Therefore, if the field or the interatomic distance R is not too large, the pair production occurs by a two-step process: (i) electrons from the negative energy sea tunnel to one of the bound state resonances, (ii) followed by an ionization process where the same electron tunnels to the positive energy continuum. This produces a flux of electron and positrons, propagating in opposite directions. There is another possibility which occurs when the RTRs from the positive and negative continua cross each other (channel 3). Then, it is possible to have a direct transition from the negative to the positive energy continua, which also enhances pair production but which effect is usually more modest than other channels because they have a lower density of states. These effects are important at a large internuclear distance R. For small R, such as in those achieved in heavy ion collisions (HIC) [18], the wave functions of each nucleus overlap and another mechanism is responsible for pair production: the effective electric charge approaches $2Z$ in which case the ground state has a lower energy level, approaching the negative energy sea. In the electric field, it is then easier for an electron to tunnel from the negative energy sea and again this also leads to enhanced pair production.

To confirm these novel ideas, a calculation of the pair production rate is performed in a very simple one-dimensional (1-D) model: the nuclei are modeled by delta function potential wells while the laser field is considered in the adiabatic limit and is taken as a static electric field. We have shown earlier that an adiabatic model which includes nonadiabatic transitions near avoided crossings is in excellent agreement with numerical results [19]. In a previous three-dimensional (3-D) model of the one electron H_2^+ molecule in superintense laser fields, it was shown how to adapt free electron Volkov solutions of the Dirac equation to the two center problem [20]. In the present work, we use a simpler model which allows us to understand the mechanisms and the physics behind the pair production from the interaction of lasers with fully ionized diatomic molecules. We show that REPP can be utilized to enhance pair production at low field strength and large internuclear distance. This conclusion is confirmed by conducting a comparative study with the cases where there are no nuclei (Schwinger's process) and where there is only one nucleus.

To calculate the average rate of pairs produced, we follow the discussion presented in Refs. [21–23] and assume that the electric field vanishes at $x = \pm\infty$ and thus, that it has a finite extent in space. In this case, it is possible to define the "asymptotic states" at $x = \mp\infty$: in these regions, the particles are free and there is a natural separation between the negative and positive energy solutions. This allows us to evaluate the number of pairs produced from a solution of the Dirac equation. It should be noted here that the boundary conditions on the wave function at $x = \mp\infty$ are obtained from the time-dependent case where the Lehmann-Symanzik-Zimmermann (LSZ) asymptotic conditions, which imply the vanishing of the field at $t = \mp\infty$, can be used [24]. In the time-independent case. however, the latter cannot be fulfilled directly: we have to consider localized wave packets which are effectively in the free region when $t = \mp\infty$. From these considerations, it is possible to evaluate the average number of pairs $\langle n\rangle$ and it has been argued in Refs. [21–23] that this observable is given by

$$\frac{d\langle n\rangle}{dtdE} = \frac{1}{2\pi}|A(E)|^2, \qquad \frac{d\langle n\rangle}{dt} = \frac{1}{2\pi}\int_{\Omega_{\mathrm{Klein}}} dE|A(E)|^2, \tag{1}$$

where A is the coefficient of the positive energy solution propagating towards $x = +\infty$, at the right of the potential (see Fig. 2) and Ω_{Klein} is the Klein region. This formula is valid for a time-independent external field where solutions are labeled by energy. Similar formulas have been derived in Ref. [25,26].

The calculation of pair production reduces to a transmission-reflection problem where the incident, reflected, and transmitted waves are given respectively by

$$\psi_{\mathrm{inc.}}(x) = v(p)e^{ip(E)x}, \tag{2}$$

$$\psi_{\mathrm{ref.}}(x) = Bv(-p)e^{-ip(E)x}, \tag{3}$$

$$\psi_{\mathrm{trans.}}(x) = Au(k)e^{ik(E)x}. \tag{4}$$

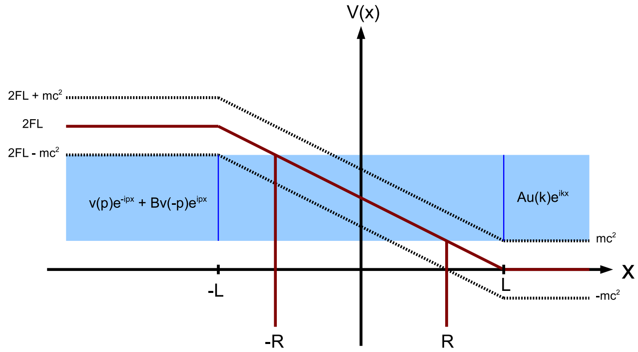

FIG. 2 (color online). Diatomic model to study REPP with $\pm R$ the positions of delta function potentials. The electric field is nonzero in $[-L, L]$. In blue is the Klein region where it is possible to have a transition from a negative to a positive energy state.

Here, u, v are the positive and negative energy free spinors, while $k(E) = \frac{1}{c}\sqrt{E^2 - m^2c^4}$ and $p(E) = \frac{1}{c}\sqrt{(E - 2FL)^2 - m^2c^4}$.

We are considering the 1-D Dirac equation, which is given by

$$E\psi(x) = [-ic\sigma_z\partial_z + \sigma_x mc^2 + A_0(x) + V(x)]\psi(x), \quad (5)$$

where E is the eigenenergy, c is the light velocity, m is the electron mass, and $\psi(x)$ is the two-component spinor wave function. The electric potential is divided in three spatial regions as (see Fig. 2)

$$A_0(x) = \begin{cases} 2FL & \text{for } x \in (-\infty, -L], \\ -F(x-L) & \text{for } x \in (-L, L), \\ 0 & \text{for } x \in [L, \infty), \end{cases} \quad (6)$$

where F is the field strength (we are working in a gauge where the vector potential is $A_x = 0$, the electric field is related to the potential as $E_x = -\partial_x A_0(x)$), and $2L$ is the length over which the electric field is constant. Outside the interval $[-L, L]$, the electric field vanishes.

For the other scalar potential, three cases are considered: (1). Zero nucleus: $V(x) = 0$ (2). One nucleus: $V(x) = -g\delta(x)$ (3). Two nuclei: $V(x) = -g\delta(x-R) - g\delta(x+R)$, where g is the potential strength (physically, it is related to the charge of the nucleus). It was shown in Ref. [17] in detail that the Dirac delta potential wells can be characterized by the following boundary conditions: $\lim_{\epsilon\to 0}\psi(\zeta+\epsilon) = \lim_{\epsilon\to 0}G\psi(\zeta-\epsilon)$ (ζ is the potential well position), which relates the wave function on the right and the left of the potential well. The matrix components are given by $G_{12} = G_{21} = 0$ and

$$G_{11} = \frac{1}{1+\frac{g^2}{4c^2}}\left[1 - \frac{g^2}{4c^2} + i\frac{g}{c}\right] = G_{22}^*. \quad (7)$$

Thus, the wave function between the potential wells is a solution of Eq. (5) without $V(x)$. Then, Eq. (7) is used to match the wave function at $x = 0, \pm R$, for cases 2 and 3, respectively.

The Dirac equation can be solved analytically by decoupling the two spinor components and by letting $y(x) = e^{-i(\pi/4)}\sqrt{\frac{2c}{F}}(\frac{E-F(x-L)}{c})$. Then, the Dirac equation becomes a system of equations with well-known solutions in terms of parabolic cylinder functions $U(\gamma, z)$ [27]:

$$\psi(x) = c_1U_a(x) + c_2U_b(x), \quad (8)$$

where $c_{1,2}$ are integration constants and where we defined

$$U_{a,1}(x) \equiv U(\gamma, y(x)) \quad (9)$$

$$U_{b,1}(x) \equiv U(-\gamma, -iy(x)), \quad (10)$$

$$U_{a,2}(x) \equiv mc\sqrt{\frac{c}{2F}}e^{i(3\pi/4)}U(\gamma+1, y(x)), \quad (11)$$

$$U_{b,2}(x) \equiv \frac{1}{mc}\sqrt{\frac{2F}{c}}e^{-i(\pi/4)}U(-\gamma-1, y(x)). \quad (12)$$

Here, we have $\gamma = i\frac{m^2c^3}{2F} - \frac{1}{2}$, which is related to the probability of producing one pair in a static field as $P_S \sim e^{i\pi(\gamma+1/2)}$ [5].

Now, imposing the continuity of the wave function at the region boundaries and using Eq. (7) to include the potential wells, we obtain the following conditions:

$$v(p)e^{ipL} + Bv(-p)e^{-ipL} = a_1U_a(-L) + a_2U_b(-L),$$
$$a_1U_a(-R) + a_2U_b(-R) = G^{-1}[b_1U_a(-R) + b_2U_b(-R)],$$
$$b_1U_a(R) + b_2U_b(R) = G^{-1}[c_1U_a(R) + c_2U_b(R)],$$
$$c_1U_a(L) + c_2U_b(L) = Au(k)e^{ipL}.$$

Similar conditions also exist for the zero and one nucleus cases. These are systems of equations which can be used to solve for the integration constants A, B, $a_{1,2}$, $b_{1,2}$, $c_{1,2}$. The numerical results are presented in the following.

The particle spectrum $d\langle n\rangle/dEdt$ as a function of interatomic distance is plotted in Fig. 3 for the two nuclei case and for $g = 0.8$ (the ground state energy of this potential well corresponds to the energy of the $1s$ orbital of the U^{91+} ion which has $E_{1s}^{U^{91+}} \approx 13908$ a.u. (1 a.u. ≈ 27 eV)). The other parameters are chosen as $L = 100$ ($\times 38.6$ pm), $F = 0.09$ ($\times 10^{18}$ V/m), in units where $\hbar = c = m = 1$ and $e = \sqrt{\alpha}$, where $\alpha = e^2/\hbar c$ is the fine structure constant. In this figure, there is a clear enhancement of pair production at the positions of resonances. Moreover, as R is varied, it is possible to see how the resonances are moving in the energy plane: some of the RTRs in the negative energy sea are shifted to higher energies while the ground state and the first excited state are Stark shifted down and up, respectively, as illustrated in the figure. More interesting is the fact that when the RTR crosses with the

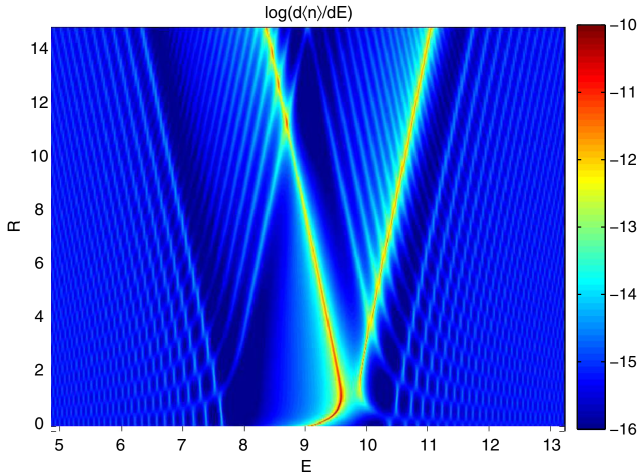

FIG. 3 (color online). Particle spectrum $d\langle n\rangle/dEdt$ for $g = 0.8$ corresponding to U^{91+}, $F = 0.09$ and $L = 100$, as a function of interatomic distance.

bound states, there is an enhancement in the pair spectrum (channel 1 or 2) by approximately an order of magnitude.

In Fig. 4, the total rate $d\langle n\rangle/dt$ for the two center diatomic model as a function of the interatomic distance is presented and compared to the zero and one nucleus nuclear potentials for two electric field strengths: $F = 0.2$ and $F = 0.09$. This figure shows clearly that the number of pairs is enhanced by REPP at larger R: the position of peaks in the rate corresponds to the interatomic distance where the ground state resonance crosses with RTRs (channel 1). This is also seen as red peaks in Fig. 3 (for example, at $R \approx 11.0$ and $E \approx 8.7$ for the first peak of $F = 0.09$). As F is lowered, the total rate is suppressed exponentially as in Schwinger's result and the crossing (for channel 1) occurs at larger R (this is because the Stark shift of the ground state resonance is $\sim -FR/2$). However, the relative enhancement (in comparison to the zero and one nucleus cases) increases and can reach approximately an order of magnitude (for $F = 0.09$). This

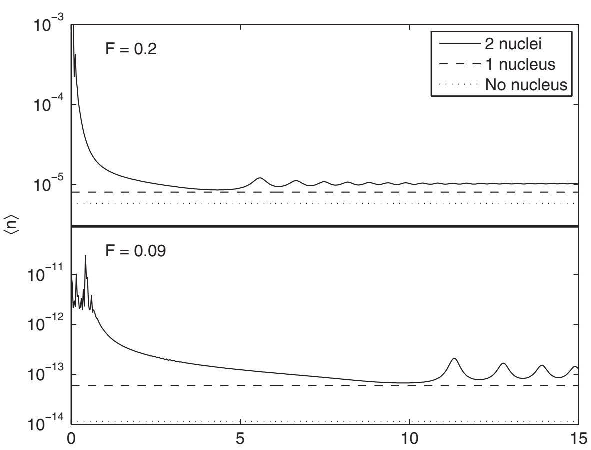

FIG. 4. Total rate $d\langle n\rangle/dE$ as a function of interatomic distance.

phenomenon is related to the fact that the density of states rises close to resonance energies as F is decreased (resonances become more stable). Therefore, REPP is an important process for pair production in laser-matter interaction.

The largest enhancement, however, occurs at small R where it reaches 2 orders of magnitude above the one nucleus case. This occurs because the effective potential strength approaches $2g$ which brings the ground state closer to the Dirac sea, facilitating the tunneling from the negative to the positive energy states. This also suggests that an experiment using HIC in a laser field could also be used to probe the Dirac vacuum, as opposed to free field experiments [18].

*filliong@CRM.UMontreal.ca
Also at School of Mathematics and Statistics, Carleton University, Ottawa, Canada K1S 5B6 and Fields Institute, University of Toronto, Toronto, Canada M5T 3J1.
†elorin@math.carleton.ca
Also at Centre de Recherches Mathématiques, Université de Montréal, Montréal, Canada H3T 1J4.
‡Andre.Dieter.Bandrauk@USherbrooke.ca
Also at Centre de Recherches Mathématiques, Université de Montréal, Montréal, Canada H3T 1J4.

[1] G. A. Mourou, T. Tajima, and S. V. Bulanov, Rev. Mod. Phys. **78**, 309 (2006).
[2] T. Brabec and F. Krausz, Rev. Mod. Phys. **72**, 545 (2000).
[3] A. D. Bandrauk and F. Légaré, in *Progress in Ultrafast Intense Laser Science VIII* of Springer Series in Chemical Physics Vol. 103, edited by K. Yamanouchi, M. Nisoli, W. T. Hill, A. W. Castleman, J. P. Toennies, K. Yamanouchi, and W. Zinth (Springer-Verlag, Berlin, 2012), ISBN 978-3-642-28726-8, pp. 29–46.
[4] Y. I. Salamin, S. Hu, K. Z. Hatsagortsyan, and C. H. Keitel, Phys. Rep. **427**, 41 (2006).
[5] J. Schwinger, Phys. Rev. **82**, 664 (1951).
[6] E. Brezin and C. Itzykson, Phys. Rev. D **2**, 1191 (1970).
[7] N. Narozhnyi and A. Nikishov, Sov. Phys. JETP **65**, 427 (1974).
[8] H. K. Avetissian, A. K. Avetissian, G. F. Mkrtchian, and K. V. Sedrakian, Phys. Rev. E **66**, 016502 (2002).
[9] M. Ruf, G. R. Mocken, C. Müller, K. Z. Hatsagortsyan, and C. H. Keitel, Phys. Rev. Lett. **102**, 080402 (2009).
[10] C. Müller, A. B. Voitkiv, and N. Grün, Phys. Rev. A **67**, 063407 (2003).
[11] A. Di Piazza, K. Z. Hatsagortsyan, and C. H. Keitel, Phys. Rev. Lett. **100**, 010403 (2008).
[12] C. Müller, A. B. Voitkiv, and N. Grün, Phys. Rev. Lett. **91**, 223601 (2003).
[13] M. Jiang, W. Su, Z. Q. Lv, X. Lu, Y. J. Li, R. Grobe, and Q. Su, Phys. Rev. A **85**, 033408 (2012).
[14] G. V. Dunne, H. Gies, and R. Schützhold, Phys. Rev. D **80**, 111301 (2009).
[15] C. K. Dumlu and G. V. Dunne, Phys. Rev. Lett. **104**, 250402 (2010).
[16] N. Milosevic, V. P. Krainov, and T. Brabec, Phys. Rev. Lett. **89**, 193001 (2002).

[17] F. Fillion-Gourdeau, E. Lorin, and A. D. Bandrauk, J. Phys. A **45**, 215304 (2012).
[18] R. Ruffini, G. Vereshchagin, and S.-S. Xue, Phys. Rep. **487**, 1 (2010).
[19] F. Fillion-Gourdeau, E. Lorin, and A. D. Bandrauk, Phys. Rev. A **86**, 032118 (2012).
[20] F. H. M. Faisal, J. Phys. B **42**, 171003 (2009).
[21] T. Damour, in *Proceedings of the First Marcel Grossmann Meeting on General Relativity*, edited by R. Ruffini (North-Holland, Amsterdam, 1977), pp. 459–482.
[22] R.-C. Wang and C.-Y. Wong, Phys. Rev. D **38**, 348 (1988).
[23] A. Hansen and F. Ravndal, Phys. Scr. **23**, 1036 (1981).
[24] A. Baltz, F. Gelis, L. McLerran, and A. Peshier, Nucl. Phys. **A695**, 395 (2001).
[25] S. P. Kim, H. K. Lee, and Y. Yoon, Phys. Rev. D **82**, 025015 (2010).
[26] A. Chervyakov and H. Kleinert, Phys. Rev. D **80**, 065010 (2009).
[27] N. Temme, in *NIST Handbook of Mathematical Functions*, edited by F. W. J. Olver, D. W. Lozier, R. F. Boisvert, and C. W. Clark (Cambridge University Press, New York, NY, 2010).