New mechanism for the generation of electron-positron pairs in Laser-Matter Interaction: Resonantly Enhanced Pair Production in a molecular system

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Abstract. A new mechanism for pair production from the interaction of a laser with two nuclei is presented. The latter takes advantage of the Stark effect in diatomic molecules and the presence of molecular resonances in the negative and positive energy continua. Both move in the complex energy plane as the interatomic distance and the electric field strength are varied. We demonstrate that there is an enhancement of pair production at the crossing of these resonances. This mechanism is studied in a very simple one-dimensional model where the nuclei are modeled by delta function potential wells and the laser by a constant electric field. The position of resonances is evaluated by using the Weyl-Titchmarsh-Kodaira theory, which allows to treat singular boundary value problems and to compute the spectral density. The rate of producing pairs is also computed. It is shown that this process yields a positron production rate which is approximately an order of magnitude higher than in the single nucleus case and a few orders of magnitudes higher than Schwinger’s tunneling result in a static field.

1. Introduction
Pair production from variations of Schwinger’s mechanism is presently a very active topic of research because it is now possible to reach laser intensities exceeding $I \sim 10^{23}$ W/cm² [1]. Although the corresponding field strength ($E = (2I/c)^{1/2}$) is still far from the “critical” Schwinger field $E_S \sim 10^{18}$ V/m, at which spontaneous emission of pairs from a static electric field becomes important, it may still be possible to observe electron-positron production by using other electric field configurations. For instance, different mechanisms have been studied such as counterpropagating lasers [2, 3, 4, 5], counterpropagating lasers with space dependence [6], the interaction of laser field with heavy nuclei [7, 8, 9, 10] and the combination of rapidly and slowly varying fields [11, 12]. The effect of the temporal laser pulse shape has also been investigated [13, 14, 15]. Most of these ideas take advantage of some of the following effects:

- Time-dependence of the laser field, which effectively shift energy levels by $\hbar \omega$ (where $\omega$ is the laser frequency).
The presence of a nucleus, which have a ground state at lower energy level than in vacuum.

Volume effects: in a laser field, pairs are produced in a bulk. Thus the small production rate (per unit volume) can be compensated by a large enough volume.

The mechanism we are proposing borrows ideas from a well-known mechanism in molecular high intensity laser physics, namely Charge Resonance Enhanced Ionization (CREI), which describes the non-perturbative ionization of diatomic molecules [16, 17]. Our main idea is to use the interaction of a laser field with a fully stripped diatomic molecule (two-center system) [18]. In this case, it is well-known that for large interatomic distance $R$ and in the presence of an electric field of strength $F$, the ground state and the first excited states are shifted in the complex energy plane: the ground and first excited states are Stark shifted by $\Delta E \sim \mp RF/2$, respectively, and they gain an imaginary part because in the field, they become unstable resonances by decaying into continuum energy states. More interesting is the fact that in such system, there are also resonances in the negative energy sea which are related to the backscattering of negative energy states on the molecular potential. These resonances are Stark shifted to higher energy by the electric field [19]. When the ground state resonance crosses one of the resonances coming from the negative energy sea, it is possible to have a transition between the negative and positive energy states resulting in an enhancement of pair production. We call this the Resonantly Enhanced Pair Production (REPP) mechanism [18] and it is depicted in Fig. 1.

In this proceeding, the REPP is studied in a very simple one-dimensional model: the two nuclei are modeled by delta function potential wells while the laser field is treated in the adiabatic regime. In this limit, we can consider a static electric field corresponding to the extrema of the field oscillations of an intense laser pulse [17, 20]. Although this model is very simple, it contains the main physical features allowing to investigate the REPP mechanism. Other 1-D models have been considered in the literature [15, 21, 14, 22].

This article is organized as follows. In Section 2, we present the model. In Section 3, we evaluate the position of resonances using the Weyl-Titchmarsh-Kodaira (WTK) theory. The pair production rate is computed in Section 4 and numerical results are in Section 5. We conclude
in Section 6. Also, units in which $\hbar = c = m = 1$ (where $m$ is the electron mass) and $\epsilon = \sqrt{\alpha}$ ($\alpha = e^2 / \hbar c$ is the fine structure constant) are utilized in numerical calculations, in comparison to atomic units where $\epsilon = \hbar = m = 1$ and $c = \alpha^{-1}$.

2. Simple diatomic model

The model considered in this work is a time-independent one-dimensional model, which allows us to compute analytical solutions. Our analysis is based on the Dirac equation as it is the basic ingredient to evaluate pair production from the “vacuum”. In the case considered, the Dirac equation is given by

$$E \psi(x) = \left[ -i c \alpha \partial_x + \beta mc^2 + V(x) + A_0(x) \right] \psi(x), \quad x \in \mathbb{R}, \quad (1)$$

where in 1-D, $\psi$ is a bi-spinor, $V$ is the scalar potential of the nuclei, $A_0(x)$ is the scalar potential of the laser field, $m$ is the electron mass and $E$ is the energy. In the first part of this work (in Section 3), where the position of resonances are evaluated in the WTK theory, it is convenient to work in a representation where the Dirac matrices are given by

Representation 1: $\alpha = -\sigma_y$ and $\beta = -\sigma_z$. \hspace{1cm} (2)

This is chosen to recover the WTK theory for systems of equations [23, 24]. In the second part of this work (in Section 4), where pair production is evaluated, it is actually more suitable to use

Representation 2: $\alpha = \sigma_z$ and $\beta = \sigma_x$, \hspace{1cm} (3)

as it yields simpler equations. Both representations obey the appropriate anticommutation relations.

The nuclei are modeled by the two center potential

$$V(x) = -g \left[ \delta(x - R) + \delta(x + R) \right], \quad x \in \mathbb{R}, \hspace{1cm} (4)$$

where $2R$ is the interatomic distance and $g$ is the strength of the Dirac delta potential wells (physically, this parameter is very similar to the electric charge of the nucleus). As in non-relativistic quantum mechanics, this type of potential can be characterized by boundary conditions at the potential well position. However, the mathematical derivation is more intricate due to the singularities because they involve the product of distributions as the wave function has a jump discontinuity ($\psi(x) \sim H(x + R) + H(x - R)$, where $H$ is the Heaviside function). Thus, the Dirac equation has terms of the form $\delta(x \pm R)H(x \pm R)$ which are not well-defined mathematically. Nevertheless, there exists a mathematical framework which includes products into the definition of distributions: the Colombeau theory of generalized functions [25, 26]. Using this theory, along with conjugation invariance and properties of self-adjoint extensions, it is possible to single out one boundary condition. In representation 1, it is given by [19]

$$\psi_1(\pm R^+) = \left[ 1 + \frac{g^2}{4c^2} \right]^{-1} \left[ \left( 1 - \frac{g^2}{4c^2} \right) \psi_1(\pm R^+) - \frac{g}{c} \psi_2(\pm R^-) \right], \hspace{1cm} (5)$$

$$\psi_2(\pm R^+) = \left[ 1 + \frac{g^2}{4c^2} \right]^{-1} \left[ \left( 1 - \frac{g^2}{4c^2} \right) \psi_2(\pm R^+) + \frac{g}{c} \psi_1(\pm R^-) \right], \hspace{1cm} (6)$$

where we defined $\psi(\pm R^+) = \lim_{\epsilon \to 0} \psi(\pm R + \epsilon)$ and $\psi(\pm R^-) = \lim_{\epsilon \to 0} \psi(\pm R - \epsilon)$. 


3. WTK theory and the position of resonances

The WTK method was developed to provide a generalization of eigenvalue expansion to singular operator\(^1\) and infinite domain, for 1-D second order equations \([27]\). This was also generalized to the 1-D Dirac equation in \([23, 24]\). This method is based on the WTK theorem which states that there exists a square integrable solution when the imaginary part of the energy \(\text{Im}(E) > 0\).

Within this framework, it is also possible to evaluate the spectral density \(\rho(E)\) which contain all the information on the spectrum of our operator: bound states appear as poles of \(\rho\) while continua occurs when \(\rho(E) \neq 0\). Resonances, which will play a very important role in the following, are poles of \(\rho\) in the complex energy plane. As these give the most relevant information from the physical point of view, we will focus on this quantity in this work.

Within the model presented in the previous section, we consider the two center problem in a static electric field which allows to describe molecular CREI in intense laser fields \([16, 17]\):

\[
A_0(x) = -Fx, \tag{7}
\]

where \(F\) is the field strength. It can be shown in the present model that the position of poles in the complex plane is obtained \([19]\) by solving numerically the equation

\[
\begin{align*}
&\left[iG_u^+ U_1^+ [a, y(R)] - G_u^- U_1^- [a, y(R)]\right] \\
&\times \left[iH_u^+ U_2^+ [a, y(-R)] - H_u^- U_2^- [a, y(-R)]\right] \\
&- \left[iH_u^+ U_2^+ [a, y(-R)] - H_u^- U_2^- [a, y(-R)]\right] \\
&\times \left[iG_u^+ U_1^+ [a, y(R)] - G_u^- U_1^- [a, y(R)]\right] = 0, \tag{8}
\end{align*}
\]

which corresponds to the spectral density denominator. Here, we have \(y(x) = e^{-i\frac{\pi}{4} \sqrt{\frac{2e}{F}} (\frac{E+Fx}{c})}\), \(a := i\frac{2e^2}{2F} - \frac{1}{2}\) and \(U_{1,2} := U_{1,2} \pm U_{1,2}\) while the other quantities are defined in Appendix A.

The numerical results for the real part of the pole position is shown in the Section 5 in Fig. 3, for \(g = 0.8\) and \(F = 0.2\).

4. Pair production rate

The pair production rate from the vacuum in a strong background static field of amplitude \(F\) is related to its corresponding Dirac equation. This physical quantity can be evaluated using the following considerations. First, we assume that the static electric field has a finite extent and is non-zero in the region \([-L, L]\). In this case, it is possible to define “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. This first assumption is required because the external field is static: in the time-dependent case, we would require the vanishing of the field at \(t = \pm\infty\).

Then, it has been argued that in the static case, the average number of pairs \(\langle n \rangle\) is given by \([28, 29, 30, 31, 32]\)

\[
\frac{d\langle n \rangle}{dt dE} = \frac{1}{2\pi} |A(E)|^2, \tag{9}
\]

where \(A\) is the coefficient of the positive energy solution propagating towards \(x = +\infty\), at the right of the potential (see Fig. 2).

\(^1\) Here, by singular, we mean that one term of the differential equation diverges on the boundary of the domain.
Figure 2: Simple model to study REPP with appropriate asymptotic particle amplitudes [18]. The electric field has a finite extent in space. In blue is the Klein region where it is possible to have a transition from a negative to positive energy states.

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

\[ \psi_{\text{inc}}(x) = v(p)e^{ip(E)x}, \]
\[ \psi_{\text{ref}}(x) = Bv(-p)e^{-ip(E)x}, \]
\[ \psi_{\text{trans}}(x) = Au(k)e^{ik(E)x}. \]

Here, \( u, v \) are the positive and negative energy free spinors in representation 2: their explicit expression will be given below.

The electric potential is divided in three spatial regions as (see Fig. 2)

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

where \( F \) is the field strength (we are working in a gauge where the vector potential is \( A_x = 0 \) and 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:

(i) No nucleus: \( V(x) = 0 \)
(ii) Single nucleus: \( V(x) = -g\delta(x) \)
(iii) Two nuclei: \( V(x) = -g\delta(x - R) - g\delta(x + R) \)

Then, Eqs. (5) and (6) are used to match the wave function at \( x = 0, \pm R \), for case 2 and 3 respectively. The Dirac equation can be solved analytically everywhere, for \( x \in \mathbb{R} \), in terms of parabolic cylinder functions.

The last missing ingredients to compute pair production are the negative and positive energy free spinors. There is a well-known procedure to compute these quantities where one seeks plane
wave solutions. This yields

\[
\begin{align*}
u(k) &= \frac{1}{\sqrt{2E}} \left[ \sqrt{E + ck(E)} \right], \\
v(p) &= \frac{1}{\sqrt{2(E - 2FL)}} \left[ \sqrt{(E - 2FL) + cp(E)} - \sqrt{(E - 2FL) - cp(E)} \right],
\end{align*}
\]  

where \( k(E) = \frac{1}{c} \sqrt{E^2 - m^2c^4} \) and \( p(E) = \frac{1}{c} \sqrt{(E - 2FL)^2 - m^2c^4} \).

Now, imposing the continuity of the wave function at the region boundaries (at \( x = \pm L \)) and using Eqs. (5) and (6) to include the potential wells, we obtain the following conditions for the three cases [18]:

(i) No nucleus:

\[
v(p)e^{ipL} + Bv(-p)e^{-ipL} = a_1U_a(-L) + a_2U_b(-L),
\]

\[
a_1U_a(L) + a_2U_b(L) = Au(k)e^{ipL}.
\]

(ii) Single nucleus:

\[
v(p)e^{ipL} + Bv(-p)e^{-ipL} = a_1U_a(-L) + a_2U_b(-L),
\]

\[
a_1U_a(0) + a_2U_b(0) = G^{-1} [b_1U_a(0) + b_2U_b(0)],
\]

\[
b_1U_a(L) + b_2U_b(L) = Au(k)e^{ipL}.
\]

(iii) Two nuclei:

\[
v(p)e^{ipL} + Bv(-p)e^{-ipL} = a_1U_a(-L) + a_2U_b(-L),
\]

\[
a_1U_a(-R) + a_2U_b(-R) = G^{-1} [b_1U_a(-R) + b_2U_b(-R)],
\]

\[
b_1U_a(R) + b_2U_b(R) = G^{-1} [c_1U_a(R) + c_2U_b(R)],
\]

\[
c_1U_a(L) + c_2U_b(L) = Au(k)e^{ipL}.
\]

Here, we defined:

\[
U_{a,1}(x) \equiv U(\gamma, y(x)),
\]

\[
U_{b,1}(x) \equiv U(-\gamma, -iy(x)),
\]

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

\[
U_{b,2}(x) \equiv \frac{1}{mc} \sqrt{\frac{2F}{c}} e^{-i\frac{\pi}{4}} U(-\gamma - 1, y(x)),
\]

where \( \gamma = \frac{mc^2}{2F} \), which is related to the probability of producing one pair in a static field as \( P_s \sim e^{\gamma(\gamma + 1/2)} \) [33], and \( U(\gamma, z) \) is the parabolic cylinder function. The system of equations obtained for each case can be used to solve for the integration constants \( A, B, a_{1,2}, b_{1,2}, c_{1,2} \) and thus, to evaluate pair production via Eq. (9). The numerical results are presented in the following.

### 5. Results

In this section, numerical results are presented. First, in Fig. 3, we show the position of resonances, obtained from the WT model, and the particle spectrum, obtained from the quantum field theory calculation. We fix the electric field to \( F = 0.2 \times 10^{18} \text{ V/m} \) and the
Figure 3: In (a), we show the position of resonances and in (b), the particle spectrum $d\langle n \rangle/dEdt$ [18], as a function of interatomic distance. The parameters are chosen as $g = 0.8$ (corresponding to $U^{91+}$), $F = 0.2$ and $L = 100$.

potential wells strength to $g = 0.8$. This value of $g$ reproduces the ground state energy of the 1s orbital of the $U^{91+}$ atom. By looking at these two pictures, it is clear that the spectrum $d\langle n \rangle/dEdt$ is enhanced when the resonances are crossing (when two lines are crossing in (a)). For instance, there is a peak in the spectrum at $E \approx 19.5$ and $R \approx 5.5$, where the ground state resonance crosses with a resonance coming from the negative energy states.

This phenomenon actually enhances the number of pair produced, which is shown in Fig. 4, for $F = 0.2$ and $F = 0.09$. The results are compared to the single and no nucleus cases. We can see a peak in $\langle n \rangle$ at the interatomic distance where the resonances are crossing (for instance, at $R \approx 5.5$ for $F = 0.2$). As the field strength is reduced, the total yield is exponentially suppressed, as in Schwinger’s result, but the relative enhancement is increased and can reach up to an order of magnitude (and maybe higher at lower field strength). We note also that the presence of resonances at small $R$ also enhances pair production because in that regime, the molecular system becomes similar to an atomic system with a net nuclear charge of $Z_{\text{eff}} \approx 2Z$. As the ground state resonance is then closer to the negative energy sea, it is easier to have a transition between the positive and negative energy states, which enhances pair production. This phenomenon could be observed in a relativistic heavy ion collision experiment where the collision region is immersed in an external electric field.

6. Conclusion
In this work, the spectral density and the position of resonances were computed for a simple model by using the WTK theory. The pair production rate was also evaluated. It was shown that there is an enhancement of positron production when the resonances from the negative energy states cross with the resonances of the positive energy states. This is the mechanism that enhances pair production at large interatomic distance and is called the REPP phenomenon.

It is interesting to estimate the intensity at which REPP starts to be important in a real molecular two center system. For the sake of this discussion, we adopt the atomic units system and we consider two uranium nuclei separated by a distance of $R = 10$ a.u.. In this more realistic case, the nuclei should be described by a Coulomb-like potential which has an infinite number of bound states in the mass gap. This is different from the potential considered in this
Figure 4: Total rate $d\langle n \rangle/dE$ as a function of interatomic distance, for $F = 0.2$ and $F = 0.09$ [18].

study which can only support two bound states. Nevertheless, REPP will proceed in a similar way as in our model because the behavior of the ground state resonance is qualitatively the same in both approaches. Of course, there can be a transition between the negative energy resonances and any of the bound state resonances, but the main contribution will come from the ground state, as we have shown in our analysis. Also, the magnitude of the enhancement depends on the potential shape and on the stability of the states subjected to the electric field. For this reason, we expect that peaks in the pair production rate for a Coulomb potential will be broader than the point-like interaction considered in this study. The energy of the ground and first excited states in this case is quasi-degenerate and is given by the ground state energy of the single nucleus case, that is $E_{\text{ground}} \approx E_{\text{exc}} \sim 13908$. a.u.. One approximate condition for REPP to occur is that the ground state reaches $-mc^2 \approx -18769$. a.u., given that its Stark shift is approximately $\Delta E \sim -RF/2$. We find that this occurs when $F \approx 6536$. a.u. = $3.36 \times 10^{15}$ V/m. This value of electric field strength corresponds to a laser intensity of

$$I_{\text{REPP}} \approx 1.5 \times 10^{24}\text{W/cm}^2,$$

as compared to atomic units of intensity, $I_0 = 3.54 \times 10^{16}\text{W/cm}^2$ and field $F_0 = 5.0 \times 10^{11}\text{V/m}$. This value of intensity is relatively close to the highest intensities reached in recent experiments [1]. It is also similar to recent estimations of the intensity at which pair production would occur in counterpropagating lasers [34] and in head-on collisions of a laser (with both high and low frequency components) with protons [10]. The present model suggests that REPP is a process that could be used to detect the production of pairs from the QED vacuum and to probe the vacuum properties in the nonperturbative relativistic regime of laser-matter interaction.

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Appendix A. Definition of functions

Here and in the following, we define

\[ U_1(a, y) := U(a, y), \]  
\[ U_2(a, y) := U(-a, -iy), \]  
\[ \tilde{U}_1(a, y) := mc \sqrt{\frac{c}{2F}} e^{\frac{i}{4} \frac{c}{c} U(a + 1, y)}, \]  
\[ \tilde{U}_2(a, y) := \frac{1}{mc} \sqrt{\frac{2F}{c}} e^{-\frac{i}{4} \frac{c}{c} U(-a - 1, y)}, \]

where \( U \) is a parabolic cylinder function. Then we have

\[ u_1(x) = c_1 U_1[a, y(x)] + c_1 \tilde{U}_1[a, y(x)] + c_2 U_2[a, y(x)] + c_2 \tilde{U}_2[a, y(x)], \]  
\[ iv_2(x) = c_1 U_1[a, y(x)] - c_1 \tilde{U}_1[a, y(x)] + c_2 U_2[a, y(x)] - c_2 \tilde{U}_2[a, y(x)], \]  
\[ v_1(x) = c_1' U_1[a, y(x)] + c_1' \tilde{U}_1[a, y(x)] + c_2' U_2[a, y(x)] + c_2' \tilde{U}_2[a, y(x)], \]  
\[ iv_2(x) = c_1' U_1[a, y(x)] - c_1' \tilde{U}_1[a, y(x)] + c_2' U_2[a, y(x)] - c_2' \tilde{U}_2[a, y(x)], \]

Letting \( y_0 := e^{-\frac{i}{4} \frac{c}{c} \sqrt{\frac{2F}{c}}} \) be the value where \( x = 0 \), the integration constants are

\[ c_1 = \frac{1}{2} \frac{U_2(a, y_0) - \tilde{U}_2(a, y_0)}{U_1(a, y_0) - \tilde{U}_1(a, y_0)}, \]  
\[ c_2 = \frac{1}{2} \frac{U_1(a, y_0) - \tilde{U}_1(a, y_0)}{U_2(a, y_0) - \tilde{U}_2(a, y_0)}, \]

and

\[ c_1' = \frac{i}{2} \frac{U_2(a, y_0) + \tilde{U}_2(a, y_0)}{U_1(a, y_0) + \tilde{U}_1(a, y_0)}, \]  
\[ c_2' = -\frac{i}{2} \frac{U_1(a, y_0) + \tilde{U}_1(a, y_0)}{U_2(a, y_0) + \tilde{U}_2(a, y_0)}, \]

Finally, we have the constants:

\[ G_u^+ := \left[ 1 + \frac{g^2}{4c^2} \right]^{-1} \left[ 1 - \frac{g^2}{4c^2} \right] u_{2,1}(R) \pm \frac{g}{c} u_{1,2}(R), \]  
\[ G_v^+ := \left[ 1 + \frac{g^2}{4c^2} \right]^{-1} \left[ 1 - \frac{g^2}{4c^2} \right] v_{2,1}(R) \pm \frac{g}{c} v_{1,2}(R), \]

\[ H_u^+ := \left[ 1 + \frac{g^2}{4c^2} \right]^{-1} \left[ 1 - \frac{g^2}{4c^2} \right] u_{1,2}(-R) \pm \frac{g}{c} u_{2,1}(-R), \]  
\[ H_v^+ := \left[ 1 + \frac{g^2}{4c^2} \right]^{-1} \left[ 1 - \frac{g^2}{4c^2} \right] v_{1,2}(-R) \pm \frac{g}{c} v_{2,1}(-R). \]

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