Interference effects in bound-free pair production in relativistic collisions of nuclei with molecules

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We consider bound-free electron-positron pair production in extreme relativistic collisions of a highly charged nucleus and a molecule. We show that, in such collisions, pronounced interference effects can arise in the emission pattern of the created positrons that are caused by the coherent interaction of the lepton field with the nuclei of the molecule.

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I. INTRODUCTION

Electron-positron pair production is an interesting quantum electrodynamical process in which energy is converted into matter particles. This process occurs with a noticeable probability if at least one of the following two conditions is fulfilled: (i) The external electromagnetic field is so strong that it is able to provide to an electron (positron) an energy of the order of the electron rest energy mc^2 on a distance of the order of the electron Compton wavelength $\lambda_C = \hbar/(mc)$, where m is the electron mass, c is the speed of light, and $\hbar$ is Planck's constant. (ii) The field varies in time so rapidly that its typical frequencies (multiplied by $\hbar$) are of the order or larger than $2mc^2$.

Examples of the most studied pair-production processes include (but are not limited to) photo pair production [1], in which a high-energy photon in the presence of a nucleus is converted into an electron-positron pair; collisional pair production [2], in which a part of the energy of two colliding charged particles is transformed into the pair; and pair production under the penetration of charged particles through crystals [3].

Theoretically, pair production was also studied for the cases of constant and uniform fields [4], slowly varying super-strong Coulomb fields [5], in colliding laser fields [6], and in collisions of a highly charged nuclei with a laser field [7].

In relativistic collisions between charged particles three different kinds of pair production are, in general, possible.

In the first one, which is termed free pair production, both the electron and positron are created as free particles. Beginning with the work of Landau and Lifshitz [2], this process has been studied in a vast amount of theoretical and experimental papers (see, e.g., [8] and references therein).

More recently, another kind of the pair-production process occurring in relativistic collisions has attracted substantial attention (see [9–14] and references therein). In this process the electron is created as a particle bound by one of the colliding nuclei and the process is called bound-free pair production. Compared to free pair production, this process is characterized by different dependencies on the collision energy and the charge of the nucleus carrying away the produced electron.

When the colliding nuclei possess charges of different signs, yet another pair-production process becomes possible in which not only the electron but also the positron is created in a bound state. This process was recently considered in [15] where it was termed bound-bound pair production. In contrast to the free and bound-free cases, the cross section for bound-bound pair production depends nonmonotonically on the collision energy and also has a different dependency on the charges of the colliding particles.

In this article we consider bound-free pair production in relativistic collisions between a highly charged nucleus and a molecule. The main focus of the present theoretical study is interference effects in the emission spectra of positrons which are produced in this process.

The wave-particle duality states that quantum objects exhibit properties of both particles and waves. Formulated almost a century ago [16] for matter particles, this concept was initially confirmed in electron diffraction experiments [17,18]. Since then, a large number of investigations have been performed in order to observe the wave nature of not only electrons but also of heavier particles such as, for example, atoms, dimers, and even fullerenes C_{60} [19]. Most of these measurements were aimed at a demonstration of Young-type double-slit phenomena, in which the coherent addition of the amplitudes of two (or more) paths, leading to interference, is related to the wave-like behavior of particles.

Starting from the work by Cohen and Fano [20], studies of Young-type interference in atomic physics have mainly focused on systems involving homonuclear molecules. Processes of ionization of and electron capture from such molecules in collisions with incident photons, electrons, and highly charged ions were intensively investigated experimentally and theoretically [21–33]. Very recently [34] interference effects were studied for the process of projectile-electron loss in fast collisions between highly charged ions and homonuclear molecules.

In the present article we explore the possibility of interference effects in the emission spectra of positrons, which are created in bound-free pair production occurring in relativistic collisions of a highly charged bare nucleus with a molecular target. These effects may arise due to the coherent scattering of the lepton field from different atomic centers of the molecule. These centers might be viewed in this case as playing the role of "slits" for the lepton field, which is rather similar to that of optical slits in the interference of electromagnetic waves.

The article is organized as follows: In the next section, based on a relativistic time-dependent perturbation approach, we derive the cross section for bound-free pair production in collisions between a nucleus and a molecule. The possibility of interference effects is demonstrated in Sec. III where we present results for the emission spectra of positrons produced in collisions of bare U^{92+} nuclei colliding with N_2 molecules.

Atomic units are used throughout except where otherwise stated.

II. GENERAL

Let us consider a collision between a highly charged projectile nucleus and a target-molecule. Let the charge of the nucleus be Z_p and let the molecule consist of atoms with nuclear charges Z_A^j ($j = 1, \ldots, N$, where N is the number of atoms in the molecule). Our consideration of the collision will be based on a simple model. This model does not describe what happens in the collision with the target, but takes into account all essential physics of the pair-production process in question.

This model is based on the Dirac sea picture in which pair production is viewed as a transition between electronic states with negative and positive total energy. We shall make the following assumptions:

First, these states are strongly influenced only by the field of the highly charged nucleus and, therefore, the electron and positron are described by the corresponding single-center Coulomb states. The field of the molecule acts merely as a collisional perturbation, which couples these states leading to pair production, and can be taken into account to first order of perturbation theory. Such an approximation is valid provided $Z_p \gtrsim Z_A^{\max}$, where $Z_A^{\max}$ is the highest nuclear charge in the molecule.

Second, the interaction between the created electron and positron may be neglected. Since the difference in the velocities of the electron and positron is typically much larger than 1 a.u., this is certainly a very good approximation.

Furthermore, we shall only consider molecules whose atoms have at least several electrons; $Z_A^j \gg 1$. The pair-production process is in general characterized by a very large (on the typical atomic scale) momentum transfer. Indeed, in the rest frame of the molecule this momentum can be roughly estimated as $\sim\eta mc^2/(v\gamma)$ where v is the collision velocity, c is the speed of light, and $\eta \gtrsim 2$. For extreme relativistic collisions, in which $v \approx c$, this yields $\eta mc/\gamma$. Under the simultaneously fulfilled conditions $Z_A^j \gg 1$ and $\eta mc/\gamma \gtrsim Z_A^{\max}$, the main contribution to the pair-production process in collisions with the molecule is given by the screening target mode, in which the lepton transition current interacts with the molecule "frozen" in its initial state [35]. Moreover, provided the condition $\eta mc/\gamma \gg Z_A^{\max}$ is fulfilled, within this mode the main contribution arises from the interaction with the unscreened atomic nuclei of the molecule. This means that, in order to treat the field produced by the molecule in the collision we can simply regard the molecule as a sum of "independent" atoms.

In the rest frame of the molecule K', its field is described by the sum of the scalar potentials of the atoms. Using results of [36] and [37], the potential created in this frame by the jth atom at the point $\mathbf{r}'$ can be taken as

$$\Phi'_j(\mathbf{r}') = \frac{Z_j \phi_j(|\mathbf{r}' - \mathbf{R}'_j|)}{|\mathbf{r}' - \mathbf{R}'_j|}, \tag{1}$$

where $\mathbf{R}'_j$ is the coordinate of nucleus of the atom, Z_j is the charge of the nucleus and

$$\phi_j(x) = \sum_l A_j^l \exp\left(-\kappa_j^l x\right). \tag{2}$$

The parameters A_j^l ($\sum_l A_j^l = 1$) and κ_j^l are tabulated in [36] and [37]. Correspondingly the scalar potential of the molecule reads

$$\Phi'_M(\mathbf{r}') = \sum_j \Phi'_j(\mathbf{r}'), \tag{3}$$

where the sum runs over all atoms constituting the molecule.

It is convenient to begin the consideration of pair production using the reference frame K in which the projectile nucleus is at rest. Once the cross section differential in the positron momentum is obtained in this frame, it can be easily recalculated into any other inertial frame.

We take the position of the projectile nucleus as the origin of K and assume that, in this frame, the center of mass of the molecule moves along a straight-line classical trajectory $\mathbf{R}(t) = \mathbf{b} + \mathbf{v}t$, where $\mathbf{b} = (b_x, b_y, 0)$ is the impact parameter, $\mathbf{v} = (0,0,v)$ is the collision velocity, and t is time. Using Eqs. (1)–(3) and the Lorentz transformation for the potentials, we obtain that the electromagnetic field of the molecule in the frame K is described by the potentials

$$\Phi_M(\mathbf{r},t) = \gamma \sum_j \Phi'_j(\mathbf{s}_j),$$
$$\mathbf{A}_M(\mathbf{r},t) = \left(0,0,\frac{v}{c}\Phi_M\right), \tag{4}$$

where $\mathbf{r} = (\mathbf{r}_\perp, z)$ is the coordinate of the point of observation of the field in the frame K, $\gamma = (1 - v^2/c^2)^{-1/2}$ is the collisional Lorentz factor, and

$$\mathbf{s}_j = (\mathbf{r}_\perp - \mathbf{b}_j, \gamma(z - vt_j)). \tag{5}$$

Here, $\mathbf{b}_j = \mathbf{b} + \delta\mathbf{b}_j$ is the impact parameter for the nucleus of the jth atom of the molecule, t_j is the time of its closest approach to the origin, and $\mathbf{s}_j$ is the vector connecting the position of the jth atomic nucleus of the molecule and the electron of the ion (as is viewed in the rest frame of the molecule).

Within first-order perturbation theory the transition amplitude for the pair production process reads

$$a_{fi}(\mathbf{b}) = -i \int_{-\infty}^{+\infty} dt \exp(i\omega_{fi}t)\langle\psi_b|\hat{W}|\psi_{\mathbf{p}}\rangle. \tag{6}$$

Here, $\psi_{\mathbf{p}}$ is the state of a created positron with a momentum $\mathbf{p}$ and the total energy ε_p. Furthermore, ψ_b is a bound state of a created electron which has the total energy $\varepsilon_b > 0$, and $\omega_{fi} = \varepsilon_p + \varepsilon_b$ is the transition frequency. Both the electron and positron move in the field of the nucleus Z_p.

The interaction between the lepton field and the molecule is given by

$$\hat{W}(\mathbf{r},t) = -\Phi_M(\mathbf{r},t) + \boldsymbol{\alpha} \cdot \mathbf{A}_M(\mathbf{r},t), \tag{7}$$

where $\boldsymbol{\alpha} = (\alpha_x, \alpha_y, \alpha_z)$ are the Dirac matrices.

It is more convenient to compute cross sections using the transition amplitude written in momentum space. Taking into account (1)–(7) and going over to this amplitude according to

$$S_{fi}(\mathbf{q}_\perp) = \frac{1}{2\pi}\int d^2\mathbf{b}\, a_{fi}(\mathbf{b}) \exp(i\mathbf{q}_\perp\cdot\mathbf{b}), \tag{8}$$

we obtain

$$\begin{aligned} S_{fi}(\mathbf{q}_\perp) &= \frac{i}{2\pi}\sum_j Z_A^j \exp[-i(\mathbf{q}_\perp\cdot\delta\mathbf{b}_j + \omega_{fi}\delta t_j)] \\ &\times \int d^3\mathbf{s}\exp(-i\mathbf{q}'\cdot\mathbf{s})\frac{\phi_j(s)}{s}\langle\psi_b|\exp(i\mathbf{q}\cdot\mathbf{r}) \\ &\times \left(1-\frac{v}{c}\alpha_z\right)|\psi_{\mathbf{p}}\rangle. \end{aligned} \tag{9}$$

In Eq. (9), δt_j is the difference in time between the closest approach to the origin by the nucleus of the jth atom and by the center of mass of the molecule, and

$$\begin{aligned} \mathbf{q} &= \left(\mathbf{q}_\perp, \frac{\omega_{fi}}{v}\right), \\ \mathbf{q}' &= \left(\mathbf{q}_\perp, \frac{\omega_{fi}}{\gamma v}\right). \end{aligned} \tag{10}$$

The cross section for pair production is obtained according to

$$\sigma_{fi} = \int d^2\mathbf{q}_\perp |S_{fi}(\mathbf{q}_\perp)|^2. \tag{11}$$

The cross section (11) takes on a very simple form if the molecule consists of two identical atoms. In such a case the cross sections σ_{fi} and $\sigma_{fi}^{(A)}$ for pair production occurring in collisions with the molecule and the corresponding single atom, respectively, are related by

$$\sigma_{fi} = 4\sigma_{fi}^{(A)}\cos^2\left(\frac{\mathbf{q}'\cdot\mathbf{l}_0}{2}\right), \tag{12}$$

where $\mathbf{l}_0$ is the vector connecting the positions of the atomic nuclei of the molecule in its rest frame. Note that, if we replace in Eq. (12) $\cos^2$ by its averaged value 0.5, we obtain the cross section in collisions with two "independent" atoms in the target molecule which differs just by a factor of 2 from the cross section for pair production in collision between the nucleus projectile and a single atom.

III. RESULTS AND DISCUSSION

Below we shall consider energy and momentum spectra of positrons created in bound-free pair production at an impact energy of 30 GeV/u. Note that the interval of collision energies ∼1 to 30 GeV/u is relevant for the future GSI facility (Darmstadt, Germany). Note also that, in our calculations of these spectra, the electron and positron are described fully relativistically by using bound and continuum Coulomb-Dirac states.

A. Positron spectra in projectile frame

We begin with the spectra in the rest frame of the projectile nucleus where they have an especially simple form and can be easily interpreted.

In Fig. 1 we present the energy spectrum of positrons produced in bound-free pair production occurring in collisions of 30 GeV/u U^{82+} nuclei with N_2 molecules (the electrons are created in the ground state of U^{91+}). The spectrum is given in the projectile frame for emission into the plane spanned by the molecular axis and projectile velocity (i.e., for $\varphi_p = 0°$). The molecular polar orientation angle is $\vartheta_M = 10°, 5°, 2°, 1°$, and $0°$. Whereas for $\vartheta_M = 10°$, the energy spectrum is already smooth (and its shape is practically identical to that produced in collisions with atomic nitrogen), it is seen in the figure that, at very small angles, the spectrum exhibits oscillations due to the alternation in the spectrum of the parts with constructive and destructive interference.

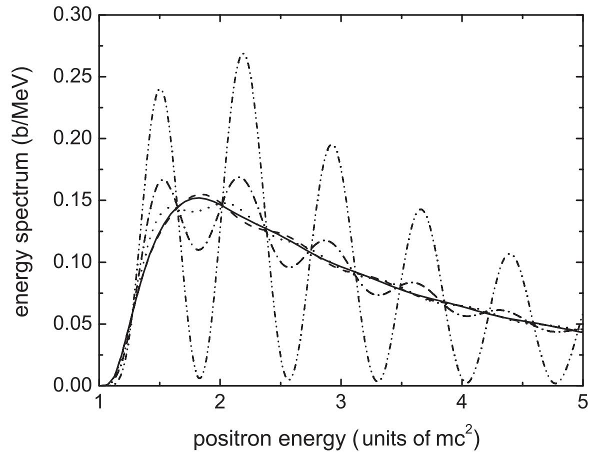

FIG. 1. Energy spectra of positrons produced in bound-free pair production in collisions of 30 GeV/u U^{92+} projectiles with N_2 molecules. The electron is created in the ground state of U^{91+}. The positrons move in the plane spanned by the molecular axis and projectile velocity. The spectra are given in the projectile rest frame. Dash-dot-dotted, dash-dotted, dotted, dashed, and solid curves correspond to $\vartheta_M = 0°, 1°, 2°, 5°$, and $10°$, respectively. The angle ϑ_M is measured with respect to the direction of the velocity $\mathbf{v}$.

The pair-production process, characterized by large momentum and energy transfers, is very well localized in position space. Even at an ultrarelativistic impact energy of 30 GeV/u ($\gamma \approx 33$), only collisions with quite small impact parameters, $b \lesssim v\gamma/\omega_{fi} \sim \gamma/(\eta c)$ ($\eta \gtrsim 2$), contribute to this process. Therefore, in order that the interaction with not just one but with both molecular centers results in pair production, the molecule has to be oriented almost parallel to the collision velocity. This is seen in Fig. 1 where only collisions at very small orientation angles ϑ_M lead to an interference structure in the energy spectrum of the produced positrons. This structure is caused by the coherent interactions (of comparable strength) between the lepton field and the two atomic centers of the molecule.

Concerning the validity of our model in the present case one can note the following: At an impact energy of 30 GeV/u ($v \approx c$) in the rest frame of the projectile nucleus, the minimum momentum transfer which is necessary to produce the pair is of the order of ηmc ($\eta \gtrsim 2$). Although, due to the Lorentz contraction, this momentum is reduced by the factor of $\gamma \approx 33$ for the target (in the target rest frame), its value nevertheless remains much larger than the typical momenta of the electrons in the molecule. This means that, within the screening-target mode, the lepton transitions are caused mainly by the interactions with the (unscreened) target nuclei. Moreover, since the momentum transfers are so large, the relative contribution to the pair-production process given by the collision mode, in which the target is excited, is about $Z_A = 7$ times smaller than that due to the screening mode. Thus, the target electrons have very little effect on the pair-production process and, therefore, the latter can be viewed as occurring due to the inelastic scattering of the lepton field from the two target nuclei. On the scale of the molecule, the nuclei are very well localized and separated from each other and play a role similar to that of two optical slits in photon diffraction.

In Fig. 2 we consider the same situation as in Fig. 1, but now by plotting the cross section for the bound-free pair-production differential in the longitudinal p_{lg} ($p_{lg} = \mathbf{p} \cdot \mathbf{v}/v$) and transverse p_{tr} ($\mathbf{p}_{tr} \cdot \mathbf{v} = 0$) components of the momentum $\mathbf{p}$ of positrons. In the figure these momentum spectra are given in the projectile frame for the emission of positrons into the plane spanned by the molecular axis and target velocity. The molecular polar orientation angle is $\vartheta_M = 10^\circ, 5^\circ, 4^\circ, 2^\circ, 1^\circ$, and 0° (from top to bottom, from left to right). Like in the case with the energy spectrum, we see that only at very small ϑ_M do the momentum spectra display clear interference. The ring-like interference pattern in the spectra corresponds to the oscillating structure of the energy spectrum of Fig. 1.

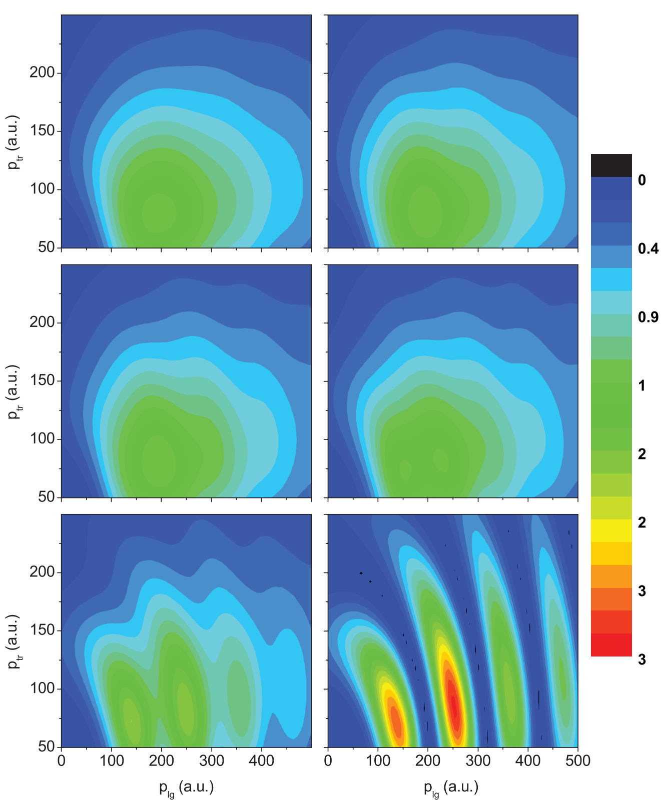

FIG. 2. (Color online) Momentum spectra of positrons produced in bound-free pair production in collisions of 30 GeV/u U^{92+} projectiles with N_2 molecules. The electron is created in the ground state of U^{91+}. The positrons move in the plane spanned by the molecular axis and projectile velocity. The spectra are given in the rest frame of the projectile and correspond (from top to bottom, left to right) to $\vartheta_M = 10^\circ, 5^\circ, 4^\circ, 2^\circ, 1^\circ$, and 0°. (Note that, in the figure, the spectra are multiplied by a factor of 100.)

B. Positron spectra in target (laboratory) frame

Now we proceed to consider positron spectra in the rest frame of the target.

In Fig. 3 we display the doubly differential cross section, $d\sigma/(d\varepsilon_p d\Omega_p)$, for bound-free pair production in collisions of 30 GeV/u U^{92+} projectiles with N_2 molecules, oriented parallel to the collision velocity (solid curves) and nitrogen atoms (dashed curves). The electron is created in the ground state of U^{91+}. The cross section is given as a function of positron energy ε_p for three different polar emission angles $\vartheta_p = 10^\circ$, 5°, and 0°. It is seen in Fig. 3 that this cross section possesses a pronounced interference pattern and thus the interference may hold also in the target frame.

However, as follows from Fig. 4, in the target frame the overall interference effects are much weaker than in the projectile frame. In this figure is shown the energy distribution of the positrons in the target frame, which is obtained by integrating $d\sigma/(d\varepsilon_p d\Omega_p)$ over the emission angles. Compared with the spectrum displayed in Fig. 1, the energy spectrum in Fig. 4 shows much weaker interference.

Such a diminishing of the interference effects could already be expected based on the results presented in Fig. 3. Indeed, the latter ones show that the positions of the maxima and minima in the doubly differential cross section depend on the angle of the positron motion. Therefore, when the integration is performed over the angle, the interference pattern is smeared out.

One should note also the following: In the projectile frame the momentum spectra of the positrons are very

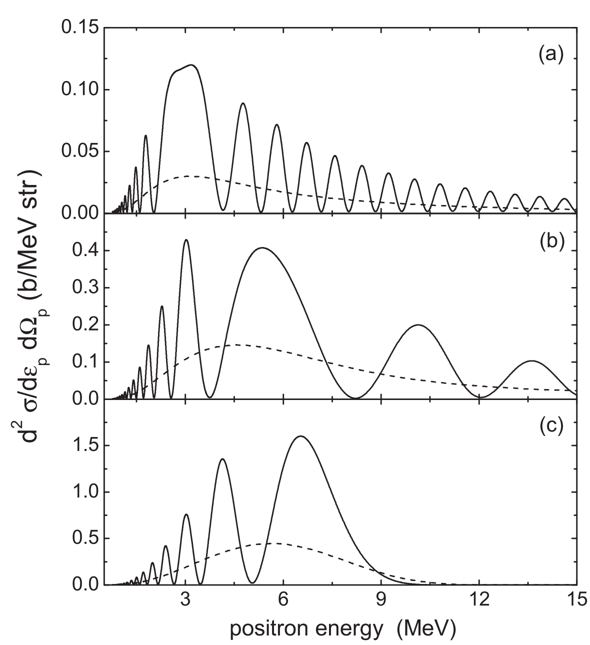

FIG. 3. Doubly differential cross section for bound-free pair production in collisions of 30 GeV/u U^{92+} projectiles with N_2 molecules, oriented parallel to the collision velocity (solid curves), and with nitrogen atoms (dash curves). The electron is created in the ground state of U^{91+}. The cross section is presented in the rest frame of the target and is given as a function of the total energy of the positron, ε_p, for a fixed value of the polar emission angle $\vartheta_p = 10^\circ$ (a), 5° (b), and 0° (c).

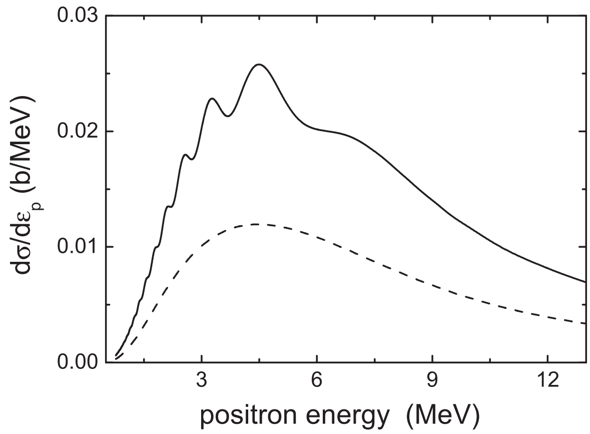

FIG. 4. Energy spectrum of positrons created in bound-free pair production in collisions of 30 GeV/u U^{92+} projectiles with N_2 molecules, oriented parallel to the collision velocity (solid curves), and with nitrogen atoms (dashed curve). The electron is created in the ground state of U^{91+}. The cross section is presented in the rest frame of the target.

asymmetric—the created positrons strongly "prefer" to move in the direction of the motion of the target. Because of that, the typical energies of the positron in the rest frame of the target are much lower than $\gamma mc^2 \approx 17$ MeV, which would correspond to positrons moving together with the projectile.

The results, shown in Figs. 3 and 4, were obtained assuming that the molecules are oriented along the projectile velocity. This is the most favorable condition for interference effects to appear. Since the positron spectra are obtained by integrating over the transverse part of the momentum transfer and the pair-production process involves very large transverse momentum transfers ($\simeq mc$) the strength of the interference is very sensitive to the deviation of the molecular orientation from the direction of the collision velocity.

In order to determine the range of molecular orientation angle ϑ_M, where the interference is clearly visible, we performed extensive calculations for the cross sections in the laboratory frame upon varying the angle ϑ_M. We found out that this range is very narrow: $\vartheta_M \lesssim 2^\circ$ to 3°. Thus, interference patterns in the positron spectra arise only at very small orientation angles of the molecule. Therefore, in order to verify predicted effects in an experiment, it is necessary to be able to single out those pair-production events, which occur at very small orientation angles, from the rest. This could, in principle, be achieved by the determination of the molecular orientation *ex post*. Such a way was rather successfully used in many experimental situations where molecular targets dissociated or Coulomb exploded after photo- and strong-field ionization or due to electron- or ion-impact-induced ionization.

IV. CONCLUSIONS

We have considered bound-free electron pair production in relativistic collisions between a highly charged bare nucleus and a molecule. In this consideration we focused on the study of interference effects in the emission of positrons. We showed that the spectra of positrons produced in such collisions may possess clear interference structures. These structures are caused by coherent interactions between the lepton field and the atomic centers of the molecule. Due to very large momentum transfers, which are characteristic for the pair-production process, this interaction is basically reduced to that between the lepton field and the nuclei of the atomic centers. Using the analogy with photon diffraction, one can say that, in our case, the interference arises from the (inelastic) scattering of the lepton field on nuclear "slits." On the scale of the molecule these "slits" are very well localized in space and distinctly separated from each other and play a role rather similar to that of the optical slits in the Young-type experiments with photons. Since the pair-production process is very tightly localized in space, clear interference structures in the spectra of produced positrons appear only in collisions at very small orientation angles of the molecule.

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