Relativistic suppression of wave packet spreading

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Abstract: We investigate numerically the solution of Dirac equation and analytically the Klein-Gordon equation and discuss the relativistic motion of an electron wave packet in the presence of an intense static electric field. In contrast to the predictions of the (non-relativistic) Schrödinger theory, the spreading rate in the field's polarization direction as well as in the transverse directions is reduced.

OCIS codes: (270.6620) Strong-field processes; (350.5720) Relativity

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#2813 - $15.00 US Received October 6, 1997

Until recently, the fully relativistic interaction of an atom with an intense laser field had been analyzed in only a few writings. A theoretical description used to compute ionization rates for hydrogen, taking into account the relativistic acceleration of electrons by the action of an intense laser source, was pioneered in large part by Reiss [1-2]. Experimental evidence indicating a deviation from non-relativistic theory and the availability of higher intensity lasers has spawned more recent studies in this area [3-6].

If one has a laser field that is sufficiently strong, theory has shown that the ionization rate of atoms can be a decreasing function of intensity [7]. Numerical simulations have also indicated that ionization in hydrogen can be suppressed by realistic laser pulses [8-10]. This stabilization has been confirmed by several research groups and has begun to stimulate experimentation [11-12]. An important question in this area concerns the fate of stabilization when relativistic effects are considered [13-18].

One can use a free electron wave packet moving in a static electric field as a first step in analyzing the relativistic corrections to the electron motion in strong laser fields [19]. Such a simplistic system allows for a clear look at purely relativistic effects while ignoring phenomena produced by the temporal characteristics of a finite laser pulse, the atomic Coulomb field and the magnetic field. We report our first results from an exact numerical solution to the Dirac equation and an analytical solution to the approximate Klein-Gordon equation.

Among our most significant findings is an alteration in the growth of the second-order moments, interpreted as a suppression in the growth of the electron wave packet's spatial width. As the electron approaches the speed of light in the long-time limit, the wave packet appears nearly frozen in the field's polarization direction. Suppression of growth in packet width is also apparent in the plane perpendicular to the polarization axis, but to a lesser extent. The role of non-relativistic wave packet spreading has been investigated in strong-field ionization [20], but the characteristics of relativistic electron wave packet spreading have never, to the extent of our knowledge, been previously discussed. We will describe the details of the subnatural spreading, the steepening of the front edge of the wave packet and a comparison with the predictions of a classical relativistic ensemble in a separate note. [21]

A static electric field $\mathbf{E}$ pointing in the x-direction acting on an electron can be described by the vector potential

$$\mathbf{A}(t) = -c\,\mathbf{E}\,t = -c\,E\,t\,\mathbf{e}_x \tag{1}$$

The motion of a quantum electron in such a field satisfies the time-dependent Dirac equation:

$$i\hbar\frac{\partial}{\partial t}\vec{\Psi}(\mathbf{r},t) = \left[mc\vec{\alpha}\left(\mathbf{p}-\frac{q}{c}\mathbf{A}(t)\right)+\vec{\beta}mc^2\right]\vec{\Psi}(\mathbf{r},t) \tag{2}$$

where $\vec{\alpha}$ and $\vec{\beta}$ are 4x4 Dirac matrices and $\vec{\Psi}(\mathbf{r},t)$ is the well-known 4-spinor [21]. A solution to this equation is made possible by discretizing the three Cartesian coordinate axes over a pre-determined volume into 64 to 512 subdivisions. A generalized split-operator Fourier algorithm was used to solve the equation in time. [21]. Our initial state used in the following calculations was:

$$\vec{\Psi}(\mathbf{r},t=0) = \left[2\pi\sigma^2\right]^{-3/4}\left(\exp\left[-(r/2\sigma)^2\right],0,0,0\right) \tag{3}$$

As in all ionization studies, the initial state of the electron is localized. This is essential to study the dynamics spatially and temporally resolved. The initial spatial uncertainty $\Delta x = \Delta y = \Delta z = \sigma$ was chosen such that the momentum width was small enough to insure that negative energy contributions (from the Dirac sea) were negligible.

Neglecting spin and possible e-p pair production, we develop an analytical description of the system. Relativistic and for now, spinless, electrons are described by a square root Klein-Gordon Hamiltonian:

$$H = \sqrt{m^2c^4 + c^2\left(\mathbf{p} - \frac{q}{c}\mathbf{A}\right)^2} \tag{4}$$

We then use our exact numerical solutions to the Dirac equation to test the validity of this approximate approach.

In analyzing the Heisenberg equations of motion, i.e. $i\hbar\frac{d}{dt}\mathbf{r} = [\mathbf{r}, H]$, we can fully solve the operator equations for the position:

$$x(t) = x + \frac{1}{qE}\sqrt{m^2c^4 + c^2(\mathbf{p} + q\mathbf{E}t)^2} - \frac{1}{qE}\sqrt{m^2c^4 + c^2\mathbf{p}^2} \tag{5a}$$

$$y(t) = y + \frac{cp_y}{qE}\ln\left\{\frac{p_x + qEt + \sqrt{m^2c^4 + c^2(\mathbf{p} + q\mathbf{E}t)^2}}{p_x + \sqrt{m^2c^4 + c^2\mathbf{p}^2}}\right\} \tag{5b}$$

$$z(t) = z + \frac{cp_z}{qE}\ln\left\{\frac{p_x + qEt + \sqrt{m^2c^4 + c^2(\mathbf{p} + q\mathbf{E}t)^2}}{p_x + \sqrt{m^2c^4 + c^2\mathbf{p}^2}}\right\} \tag{5c}$$

The momentum operators are conserved over time since the Hamiltonian of Eq. (4) commutes with each of the canonical momenta p_x, p_y and p_z. From the time derivative of Eqs. (5), one can easily see that $\dot{y}$ and $\dot{z}$ go to 0 while $\dot{x} \to c$. The motion in the plane perpendicular to the polarization axis of the field is altered although there is no force in that plane. This deceleration is a simple consequence of the fact that the speed $v(t) = \sqrt{\dot{x}^2 + \dot{y}^2 + \dot{z}^2}$ cannot attain the speed of light c. As the electron is accelerated in the x-direction, it must slow down in the y- and z-directions.

The second-order moment is defined by

$$\Delta x^2 = \left\langle \left(x - \langle x \rangle\right)^2 \right\rangle \tag{6}$$

for x and in the same way for y and z. Our notation is simplified, if we restrict our analysis to symmetric initial states here: $\Psi(\mathbf{r}, t=0) = \Psi(-\mathbf{r}, t=0)$ and $\phi(\mathbf{p}, t=0) = \phi(-\mathbf{p}, t=0)$.

The time evolution of the width is determined by all higher-order moments of the momentum because of the square root of the operators in the expectation values at t=0. In the nonrelativistic limit these equations reduce to $\Delta x_{NR}(t)^2 = \Delta x^2 + \Delta {p_x}^2 t^2 / m^2$ for x and similarly for y and z.

The relativistic case is of interest in the long-time limit:

$$\Delta x^2(t \to \infty) = \Delta x^2 + \frac{1}{q^2E^2}\left[c\left\langle p_x^2 + \mathbf{p}^2\right\rangle + m^2c^4\right] - \frac{1}{q^2E^2}\left\langle\sqrt{c^2\mathbf{p}^2 + m^2c^4}\right\rangle^2 \tag{7}$$

A logarithmic divergence occurs in the spatial variances for the transverse directions according to $\Delta z(t \to \infty)^2 = \Delta z^2 + \frac{c^2\langle p_z^2\rangle}{q^2E^2}\ln^2\left[\frac{2qEt}{mc}\right]$ for the z-direction. The spreading rate undergoes

#2813 - $15.00 US
Received October 6, 1997

a significant reduction as the electron approaches the speed of light and the spatial probability distribution is frozen in the x-direction. If we assume all velocity contributions in the initial state to be negligible in comparison to the speed of light, i.e. a wave packet initially at rest, Eq. (7) can be reduced to

$$\Delta x^2(t \to \infty) = \Delta x^2 + \frac{c^2 \langle p_x^2 \rangle}{q^2 E^2} \tag{8}$$

and directly interpreted. A nonrelativistic particle initially at rest takes a time $t^* = \frac{mc}{qE}$ to exceed the speed of light. The wave packet spreads as it is accelerated according to the nonrelativistic formula $\Delta x_{NR}(t)^2 = \Delta x^2 + \Delta p_x{}^2 t^2 / m^2$. When t=t*, we obtain Eq. (8) for the relativistic width. Using this reasoning, we could conclude that the Schrödinger theory would roughly agree with the relativistic theory up to t=t*. We would also expect the final width to be proportional to 1/E because the electron approaches c more quickly and has less time to spread for stronger E fields.

We continue with a graphical depiction of our results. To ease in this representation, we adopt atomic units with $|q| = \hbar = m = 1$ and $c \approx 137$. Our initial state is the first component of (3) and we choose E=1000 a.u. (ca. 5×10^{12}V/cm), meaning t*=0.137 a.u. The square root expectation values in Eqs. (6) were evaluated numerically in Fourier space.

Figure 1 is a plot of the variance in each of the three coordinate directions as predicted by relativistic Klein-Gordon theory Eqs. Also in this figure is the variance according to nonrelativistic Schrödinger theory for which $\Delta x_{NR}(t) = \Delta y_{NR}(t) = \Delta z_{NR}(t)$. The predictions agree for short times but soon begin to diverge. As the electron approaches the speed of light, the spreading rate in all three spatial directions is severely retarded. In fact, spreading in the x-direction approaches the value $\Delta x(t \to \infty) =$ 0.6935 from Eq. (8) and in the transverse directions is reduced logarithmically.

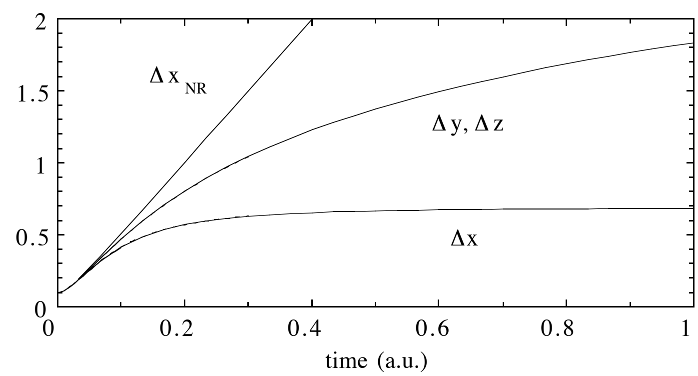

Fig. 1. The graphs show the temporal growth pattern of the spatial width obtained from Eqs. (6) Δx(t), Δy(t) and Δz(t) together with the non-relativistic width $\Delta x_{NR}(t)$. Superimposed on the graphs for Δx(t), Δy(t) and Δz(t) are the width determined from the time-dependent wave function solution obtained from the full Dirac equation Eq. (2) (dash lines). The two graphs are indistinguishable. [E=1000 a.u., initial quantum state as in Eq. (3) with σ=Δx(t=0)=0.1 a.u.]

Figure 1 also serves to compare our (approximate) theoretical results obtained from the Heisenberg equations of the (approximate) Klein-Gordon Hamiltonian and our (exact) numerical results obtained by a full solution to the Dirac equation. Limits on our grid size for the numerical solution caused by memory restrictions made it possible to trace the time evolution of the Dirac wave packet only to t=0.3 a.u. The spatial variances calculated from this wave packet are in superb agreement with the widths predicted by the Heisenberg

#2813 - $15.00 US Received October 6, 1997

equations. The approximate relativistic Klein-Gordon theory used for an analytical analysis agrees with our exact Dirac results (dashed lines) as well. After projecting our wave function on the negative energy eigenstates, we found that throughout the entire interaction, the population in the Dirac sea stayed at negligible levels. In addition, the monotonic time evolution of the first order moment (not presented) also confirms that effects due to the Zitterbewegung are not so important here.

Figure 2 shows the spatial profiles of our Dirac wave packet in both the x- and z-directions.

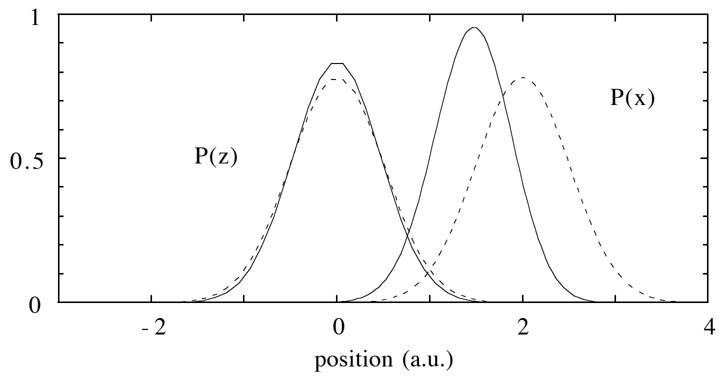

Fig. 2. Displayed are the spatial probability distributions $P(x,t) \equiv \sum_i \int dydz \left|\Psi_i(x,y,z,t)\right|^2$ and $P(z,t) \equiv \sum_i \int dxdy \left|\Psi_i(x,y,z,t)\right|^2$ in the x- and z direction at time t=0.1 a.u. For comparison, the dashed lines show the corresponding distributions obtained from the non-relativistic Schrödinger time evolution. The initial wave packet was centered initially at $\mathbf{r}$=(–3, 0, 0) for better graphical clarity. The non-relativistic wave packet has moved to x(t=0.1a.u.) =–3a.u. + $Et^2/2$ = 2.a.u. [Same parameters as in Fig. 1]

We can explain the observed suppression in wave packet spreading if we investigate how the velocity distribution changes with time. In nonrelativistic theory the velocity distribution remains shape invariant and only the position of the center changes. The velocity distribution must narrow as the velocity goes to c and the effective acceleration decreases. As t increases, the velocity distribution approaches a peak at c with zero (velocity) variance. Since spatial spreading is a direct consequence of a the dispersion in velocities, it follows that a reduction in the velocity variance should signify a decrease in spreading. It is important to note here that the zero width in velocity accompanied with a finite width in real space does not violate any quantum uncertainty relation. The product of the two uncertainties $\Delta\dot{x}\Delta x$ has no positive lower bound. The usual uncertainty product $\Delta p_x\ \Delta x$, however, grows as a function of time as the canonical momentum is conserved under the time-evolution.

Acknowledgment

We acknowledge several useful discussions with S.D. Hassani. We have also benefited from conversations with A. Belkacem, J.H. Eberly, M.V. Fedorov, H.R. Reiss. Technical assistance from undergraduate students J.W. Braun and J.C. Csesznegi is acknowledged. This work has been supported by the NSF under grant PHY-9631245. We also acknowledge support from the Research Corporation for Cottrell Science Awards and ISU for a URG. BS thanks the Illinois State University Honors Program for support of his undergraduate research work.

#2813 - $15.00 US Received October 6, 1997