Quantum signatures in laser-driven relativistic multiple-scattering

Guido R. Mocker† and Christoph H. Keitel‡

Theoretische Quantendynamik, Physikalisches Institut, Universität Freiburg,
Hermann-Herder-Straße 3, D-79104 Freiburg, Germany

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The dynamics of an electronic Dirac wave packet evolving under the influence of an ultra-intense laser pulse and an ensemble of highly charged ions is investigated numerically. Special emphasis is placed on the evolution of quantum signatures from single to multiple scattering events. We quantify the occurrence of quantum relativistic interference fringes in various situations and stress their significance in multiple-particle systems, even in the relativistic range of laser-matter interaction.

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The interplay of the strongest forces in atomic physics via ultra intense laser pulses and highly charged ions is governed rather well by quantum relativistic Dirac dynamics \[1,2,3\]. On one hand, for single particles quantum effects such as tunneling, spin effects and quantum interferences have shown to be rather crucial even in the regime of ultra-short and highly relativistic dynamics \[4,5\]. On the other hand, for many particle systems, laser-induced plasma physics was shown to be remarkably well described by classical relativistic dynamics \[6,7\]. With the intermediate regime from few particle to cluster physics attracting increasing interest \[8\], the question arises for the role of quantum effects in laser-induced relativistic dynamics.

In this letter we investigate the quantum relativistic dynamics of laser-driven multiple-scatterings of an electron being represented by a Volkov wave packet at an ensemble of highly charged ions. With an numerical accuracy, which allows for transitions even to the Dirac sea with negative energies, we quantify the interference fringes at each scattering event and the mutual interplay among those events. Clear quantum behaviour in the fringes at each scattering event and the mutual interplay is identified in the highly relativistic regime after multiple scattering.

The system of interest consists of an electron which is driven by an intense laser pulse with time \(t\) and space \(\vec{r}\) dependent vector potential \(\vec{A}(t, \vec{r})\) and scattered multiply at an ensemble of ions with scalar potential \(A_0(\vec{r})\). The electronic wave packet dynamics in such an environment is characterised by the Dirac spinor \(\psi(t, \vec{r})\) and is governed by the Dirac equation reading in atomic units as throughout the article:

\[
\frac{i\hbar}{\partial t}\frac{\partial \psi}{\partial t} = \left[ \frac{\hbar c}{i} \alpha^j \frac{\partial}{\partial r^j} + \beta mc^2 + q \left( A_0 - \alpha^j A_j \right) \right] \psi \quad (1)
\]

with electron charge \(q = -1\) a.u., electron mass \(m = 1\) a.u. and \(\alpha^j (j \in \{1, 2, 3\})\) and \(\beta\) being the Dirac matrices

\[\begin{align*}
\alpha^1 &= \begin{pmatrix}
0 & 1 \\
1 & 0
\end{pmatrix}, & \alpha^2 &= \begin{pmatrix}
0 & -i \\
i & 0
\end{pmatrix}, & \alpha^3 &= \begin{pmatrix}
1 & 0 \\
0 & -1
\end{pmatrix}, & \beta &= \begin{pmatrix}
0 & 1 \\
1 & 0
\end{pmatrix}.
\end{align*}\]

The three components of \(\vec{r}\) and \(\vec{A}\) are \(r^j\) and \(A^j\), respectively, and \(c = 137.036\) a.u. the speed of light.

Our numerical analysis takes advantage of splitting the linear Dirac Hamiltonian into a position-dependent and a derivative-dependent part. We then make use of the so-called “split-operator” technique \[10\], in which we propagate the wave packet successively by the position- and derivative-dependent parts and employ fast-Fourier-transformations, such that all operations are plain multiplications. With time step \(\Delta t\), the numerical error introduced this way is of the order \(\Delta t^3\) \[11\]. For \(\Delta t \approx 2 \times 10^{-5}\) a.u. \(< \frac{\hbar}{2mc}\), transitions between positive- and negative-energy states are resolved, and this way we obtained convergence of our split-step propagation of \(\psi\) even at large \(t \gtrsim 10\) a.u.. Further the spacing of the grid in position space needs to be suitable to resolve the maximal momenta employed. In spite of large relativistic velocities, this is not problematic, because it is the canonical rather than the kinetic momentum that has to be represented on the grid, with \(\vec{p}_{\text{can}} - \frac{2}{\beta} \vec{A} = \vec{p}_{\text{kin}}\). In the case of a high velocity of the particle being exclusively due to an intense laser field, \(\vec{p}_{\text{can}}\) is even zero in polarization direction. It is non-zero in propagation direction, but its magnitude is small even for intense fields. Once scatterings with nuclei have occurred, however high canonical momenta appear, which, for the parameters used here, can be represented successfully on a grid with a spacing \(\Delta x_i = 0.118\) a.u., corresponding to a maximum momentum of 26.6 a.u.. The so-called fermion doubling problem, which occurs at momenta close to the highest grid momenta, is consequently also avoided \[11\].

For the sake of reducing computing power, we introduced two advantageous techniques. Firstly, in position space, the calculation is restricted to the area centered around the rapidly moving wave packet, involving a “moving-grid” approach. Secondly, the grid size, too, is dynamically adapted in time: While a freely evolving wave packet spreads with time, a multiply scattered one does considerably more. As our simulation has to cover a substantial part of the whole laser pulse, including times where the packet is still quite small, it is possible to save considerable CPU time, noting that the time consuming two-dimensional fast-Fourier-transformations scale as \(N^2 \log N\), where \(N \times N\) equals the grid size. This

*Electronic address: mocken@physik.uni-freiburg.de
†Electronic address: keitel@uni-freiburg.de

URL: \url{http://tqd1.physik.uni-freiburg.de/~chk/a11/index_de.html}
“growing-grid” approach is also our pragmatic solution to the well-known boundary problem \[^{3}^{12}\] in Dirac calculations, at least to the point where damping functions and absorbing boundaries become unavoidable. Finally, the whole code is written to take advantage of multiple CPUs.

In a series of contour plots, we present the time evolution of an initially Gaussian shaped wave packet under the influence of a strong laser pulse, which is subsequently scattered at several highly charged ions. We use a four cycle laser pulse with amplitude \(E_0 = 50\) a.u. \((I = 8.75 \times 10^{19}\, \text{W/cm}^2)\) and frequency \(\omega = 1\) a.u., which features a 1.5 cycles \(\sin^2\) turn-on and turn-off, and one cycle of constant intensity in between. As amplitude and frequency suggest, we are clearly in the fully relativistic regime. The ions are modeled by static softcore potentials \(Z e^2 / \sqrt{(r - \vec{r}_{\text{ion}})^2 + a}\), with a “Coulomb-like” small softcore parameter \(a = 0.01\) being just large enough to avoid numerical instabilities at the ions’ origins \(\vec{r}_{\text{ion}}\). We chose their charge as a high multiple \((Z = 50)\) of the elementary charge \(e\) in order to acquire comparable field strengths for laser and ions (at 1 a.u. distance from the ionic center).

In fig. 11 the top left graph illustrates an overview of the successive quantum relativistic scattering scenario of an electron wave packet at two highly charged ions. The
initial Gaussian wave packet (positive energy and spin up only) is centered around the origin and its evolution is depicted by various snap shots along its center of mass motion (solid line) in the laser pulse. At first, after a short motion in the negative polarization and positive propagation directions during the first half cycle of the turn-on phase, the particle is visibly accelerated in the polarization direction, reaching the first upper turning point after the first whole cycle is completed. Further on, continuing with a clear Lorentz-force induced drift in the laser propagation direction, reaching the first upper turning point after phase, the particle is visibly accelerated in the polarization direction. The fringes maintain their orientation in various sub-wave packets, continues in positive polarization direction. The fringes would be observed and calculate the correspondence of an ion at $\mathbf{r}_{\text{ion}} = 0$, we obtain

$$
\psi(\mathbf{r}) = \phi(\mathbf{r}) - \int d^3r' G_0(\mathbf{r}, \mathbf{r}'; E) V(\mathbf{r}') \psi(\mathbf{r}') \tag{2}
$$

with unperturbed Dirac wave $\phi(\mathbf{r}) = \omega^\rho(\mathbf{p}) e^\frac{\mathbf{p} \cdot \mathbf{r}}{\hbar}$ ($\rho \in \{1, 2\}$), corresponding eigenvalue $E$ and $\omega^\rho(\mathbf{p})$ being the free-electron spinor amplitude. On the right hand side of eq. (2), we replace $\psi$ by $\phi$ (first Born approximation) and insert the relativistic free-particle Green’s function at energy $E$ [14]

$$
G_0(\mathbf{r}, \mathbf{r}'; E) = \frac{1}{\hbar c} \left[ \hat{\mathbf{\alpha}} \cdot \mathbf{p} + \beta mc^2 + E \right] e^{\frac{e^\mathbf{p} \mathbf{r}}{\hbar c^2}} \quad \text{for } |\mathbf{p}| \ll c \quad \text{and } E \ll mc^2.
$$

where $R = |\mathbf{r} - \mathbf{r}'|$, $p = \sqrt{\mathbf{p}^2 - (mc)^2}$, $\mathbf{p} = -i\hbar \nabla$, $\mathbf{p}$ the initial momentum, $\mathbf{p}' = \mathbf{p} - \mathbf{r}'$ the final momentum and $p = \hbar k = |\mathbf{p}| = |\mathbf{p}'|$ its magnitude. For the case of interest $r \gg r'$, neglecting contributions of order $\frac{1}{r}$ and higher, and assuming a short-range potential, one finally obtains the outgoing electronic wavefunction

$$
\psi(\mathbf{r}) = \omega^\rho(\mathbf{p}) e^\frac{\mathbf{p} \cdot \mathbf{r}}{\hbar} \cdot \mathbf{r} + \frac{1}{4\pi^2 \hbar c^2} \left[ \hat{\mathbf{\alpha}} \cdot \mathbf{p}' + \beta mc^2 + E\mathbf{p}' \right] \int d^3r' V(\mathbf{r}') \omega^\rho(\mathbf{p}) e^{\frac{e^\mathbf{p} \mathbf{r}}{\hbar c^2}} \cdot \mathbf{r}'. \tag{4}
$$

We are interested in the maxima of $|\psi|^2 = \psi^\dagger \psi$, or more exactly in the angles $\vartheta_n$ that point towards the scattering fringes. Using $V(\mathbf{r}') = -V_0 \delta(\mathbf{r}')$ [13] with $V_0 > 0$ as the simplest potential, we finally obtain, up to an additive function $f(r)$ and a constant pre-factor, the $\vartheta$-dependant part of $|\psi|^2$ as

$$
|\psi|^2 \propto \left( (\gamma^2 - 1) \cos \vartheta + 1 + \gamma^2 \right) \cos (kr - k r \cos \vartheta) + f(r). \tag{5}
$$

In the nonrelativistic case $\gamma = \frac{E_{\text{kin}}}{E_{\text{kin}}} \approx 1$, the maxima of the above expression can be simplified further to read

$$
\vartheta_n = \pm \arccos \left( 1 - \frac{n \pi}{kr} \right), \quad n \in \mathbb{N}. \tag{6}
$$

Then to adapt the dynamics in the laser fields, one may choose for a fixed initial momentum $\hbar k$ a distance $r$ where, in the absence of a laser field, the scattering fringes would be observed and calculate the corresponding angles $\vartheta_n$. Then with the laser field and, using a classical formula [13] and now neglecting the ionic potentials, one may propagate over a period $t = \frac{m}{e} \Delta t$ a suitably chosen ensemble of classical particles that initially starts at
FIG. 2: a) Overview: Contour plots at time $t = 12.270$ a.u. after two scatterings at an ensemble of six $\text{Sn}^{50+}$ ions (thick dots) centered symmetrically around a further one at position $(0, 30)$ a.u.. The dashed rectangle marks the grid boundary and the solid line depicts the trajectory of the expectation value of the electron’s spatial coordinate. b) This enlarged view of the wave packet in a) illustrates how the two scattering events at seven ions modify the regularity in the interference pattern. Contour lines are shown for $|\psi|^2$ with log $|\psi|^2 \geq -4$ and line spacings marking steps of 0.15.

the position of the scattering center with initial momenta of magnitude $\hbar k$ in the direction of the scattering angles $\vartheta_n$. This simple model qualitatively confirms our numerical results while it predicts the final positions and separations of the fringes by better than a factor of two. In addition to the stressed approximations in the analytical approach, mimicking the quantum wave packet in the transition regime from scattering to free dynamics in the laser field is too delicate to compete seriously in accuracy with the up-initio quantum relativistic approach.

Concluding, relativistic quantum dynamics was investigated for a multiple-particle system with clear interference fringes being identified and quantified. While quantum signatures in many-particle systems are likely to be washed out, our examples show that there is an intermediate regime in the number of involved particles with clear quantum effects for relativistic dynamics.

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