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Solution of relativistic quantum optics problems using clusters of graphical processing units

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ABSTRACT

Numerical solution of relativistic quantum optics problems requires high performance computing due to the rapid oscillations in a relativistic wavefunction. Clusters of graphical processing units are used to accelerate the computation of a time dependent relativistic wavefunction in an arbitrary external potential. The stationary states in a Coulomb potential and uniform magnetic field are determined analytically and numerically, so that they can used as initial conditions in fully time dependent calculations. Relativistic energy levels in extreme magnetic fields are recovered as a means of validation. The relativistic ionization rate is computed for an ion illuminated by a laser field near the usual barrier suppression threshold, and the ionizing wavefunction is displayed.

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1. Introduction

Tunneling ionization is usually described using the time dependent Schrödinger equation (TDSE). The TDSE is a strictly non-relativistic equation. In contrast, the dynamics of a free particle become relativistic when the normalized vector potential, $a = eA/mc^2$, satisfies $a \gtrsim 1$. For typical laser frequencies, this corresponds to an irradiance $I \approx 10^{18}$ W/cm^2. Such irradiances are achieved regularly in many laboratories. The corresponding fields are sufficient to strip nitrogen down to the K-shell via barrier suppression. Irradiances of $I > 10^{20}$ W/cm^2 are not achieved as frequently, but are easily within the reach of several ultra-high power laser systems around the world. It is expected that these irradiances are sufficient to fully strip neon.

Although the dynamics of free electrons are relativistic for $a \gtrsim 1$, the spectra of atoms that can be brought to a high charge state by such a field are non-relativistic. Put another way, all the bound electrons in an atom that requires $a \gtrsim 1$ to be fully stripped, are well described by Schrödinger theory. To see this, note that for a hydrogen-like ion, the barrier suppression model [1] gives the threshold for ionization as

$$a = \frac{\alpha}{\omega_L \tau_a} \frac{Z^3}{16} \tag{1}$$

where Z is the atomic number, ω_L is the laser frequency, $\tau_a = \hbar^3/me^4$ is the atomic unit of time, and $\alpha = e^2/\hbar c$ is the fine structure constant. Taking $a = 1$ and a laser wavelength $\lambda = 0.8$ μm ($\omega_L \tau_a = 0.057$) gives $Z = 5$. Hence, boron is the heaviest element that is fully stripped by a laser with $\lambda = 0.8$ μm and $a = 1$. The condition for an atomic spectrum to be non-relativistic is $Z \ll \alpha^{-1} \approx 137$, as follows from elementary Dirac theory. One concludes that even though $a = 1$ leads to

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relativistic motion of free electrons, the bound electrons that are freed are non-relativistic. This observation can be useful when formulating the initial conditions for a relativistic quantum optics problem.

The process of ionization involves the dynamics of both bound and free electrons. For $a \gtrsim 1$ and $Z \ll 137$, the bound electrons are quantum mechanical and non-relativistic, while the free electrons are relativistic and classical. If much heavier elements are considered, even the bound electrons might have to be treated relativistically. Hence, a complete description of the problem must be quantum mechanical and fully relativistic. In this paper we develop a numerical tool capable of treating such problems.

The non-relativistic theory of photo-ionization was pioneered by L.V. Keldysh in 1965 [2]. Shortly thereafter, in the series of papers by Perelemov et al. [3–6], it was brought into a form that has remained useful right up to the present day. Numerical solution of the non-relativistic ionization problem has been tractable for some time, although new algorithms are still being developed [7–9], including some that utilize graphical processing units [10–12]. Relativistic photo-ionization has received less attention, although some analyses have been given [13–16]. Fully time dependent numerical solutions of relativistic wave equations are only recently appearing in the literature [17–19].

2. Relativistic wave equations

The Dirac equation describes the motion of an electron in an external potential, such as the superposition of an atomic binding potential and a laser field. Solution of the Dirac equation requires evolving a 4-component bi-spinor wavefunction. However, as discussed in Ref. [20], the Dirac equation can be separated into 4 independent equations by neglecting terms involving spin. This results in the Klein–Gordon equation

$$\left[(\imath\partial_t + q\Phi)^2 - (\imath\nabla + q\mathbf{A})^2 - m^2\right]\Psi = 0 \tag{2}$$

where q is the charge, m is the mass, Φ is the scalar potential, $\mathbf{A}$ is the vector potential, and Ψ is a complex scalar wavefunction. Here, and in all that follows, natural units are employed, with energy normalized to the electron mass. Using the Coulomb gauge, $\nabla\cdot\mathbf{A} = 0$, and assuming a static scalar potential,

$$\left(\Box^2 - m^2 + q^2 A_\mu A^\mu\right)\Psi + 2\imath q\partial_\mu\left(A^\mu\Psi\right) = 0 \tag{3}$$

where $\Box^2 = \nabla^2 - \partial_t^2$, μ is a relativistic tensor index, and the metric signature is $(+---)$. Note that in the chosen gauge $\nabla\cdot(\mathbf{A}\Psi) = \mathbf{A}\cdot\nabla\Psi$. The expression on the left is useful for finite volume differencing, while the one on the right is useful for analysis.

Depending on the problem, various coordinate systems are used to solve Eq. (3). Consider Cartesian coordinates (x, y, z), cylindrical coordinates (ρ, φ, z), and spherical coordinates (r, θ, φ). Cartoons of various wavefunctions are shown in Fig. 1. Panels (a), (b), and (c) are for a central binding potential $\Phi(r)$, while (d), (e), and (f) are for a cylindrical binding potential $\Phi(\rho)$. Naturally, the former case is a more realistic model of an atom or ion. Panels (a) and (d) show a bound state wavefunction for which $\mathbf{A} = 0$. In both geometries, two coordinates are ignorable. Panels (b) and (e) show an ionizing wavefunction is the non-relativistic dipole approximation, where $\mathbf{A} = \mathbf{A}(t)$ is a function of time only. The effect of the vector potential is to stretch the wavefunction in the polarization direction. For a central potential, φ is ignorable, while for a cylindrical potential z is ignorable. Panels (c) and (f) show an ionizing wavefunction in the relativistic case, where the spatial dependence of $\mathbf{A}$ leads to a ponderomotive force that stretches the wavefunction in the direction of the photon momentum, $\mathbf{k}$. In this case, there is no coordinate that is ignorable for a central potential, but there is one that is ignorable for a cylindrical potential. This is the reason for considering a cylindrical potential.

3. Stationary states

In the remainder of this paper, cylindrical atoms are considered. The stationary states are characterized by two quantum numbers: the radial quantum number, $n_r \in \{0, \mathbb{N}\}$, and the magnetic quantum number, $\ell_z \in \mathbb{Z}$. A given stationary state is denoted $|n_r, \ell_z\rangle$.

3.1. Coulomb potentials

The time independent form of Eq. (3) is obtained by making the substitution $\Psi(\mathbf{r}, t) \to R(\rho, z)\exp(\imath\ell_z\varphi)\exp(-\imath\omega t)$. Using $\partial_t\Phi = 0$, and specializing to the case of a uniform magnetic field $\mathbf{A} = \frac{1}{2}\rho B_0\mathbf{e}_\varphi$, gives

$$\left(\nabla^2 - \omega^2 + 2q\Phi\omega + q^2\Phi^2 + \ell_z q B_0 - \frac{1}{4}\rho^2 q^2 B_0^2 - m^2\right)R(\rho, z) = 0 \tag{4}$$

In the case of a Coulomb potential, $\Phi = Q/\rho$, the bound states can be determined analytically. If the magnetic field is weak, the B_0^2 term can be dropped, and the energy levels become

$$\omega = m\left(1 - \frac{\ell_z\omega_c}{m}\right)^{1/2}\left[1 + \frac{Q^2q^2}{(n_r + \frac{1}{2} \pm \sqrt{\ell_z^2 - Q^2q^2})^2}\right]^{-1/2} \tag{5}$$