Nonlinear response of 1D multi-level system calculated from nonstationary Shrödinger equation

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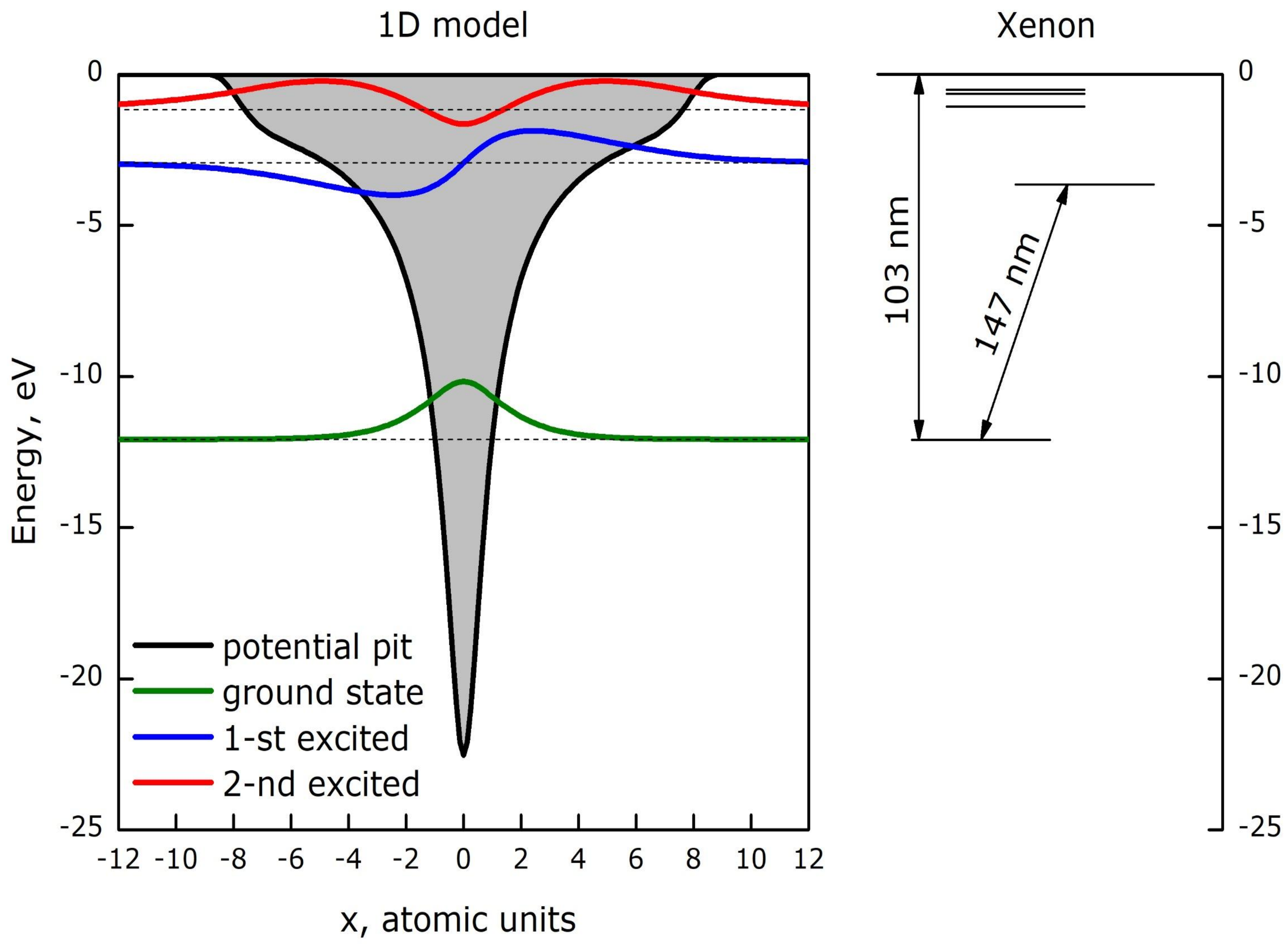
Abstract

Theoretical description of filamentation in transparent media widely relies on nonlinear propagation equations like UPPE, NLSE, etc [1]. The nonlinear response of the medium is usually considered as independent additive responses of bound electrons (3rd and higher order polarization) and self-induced plasma calculated according to rate equations. Such a method provides only limited possibilities to account for the dispersion of nonlinearity, i.e. the dependence of nonlinear coefficients on the frequency of the optical pulse, which is important for the multi-harmonic pulses or ultraviolet pulse propagation. To provide the description of this dispersion, a quantum approach is desirable.

However, full-scale 3D-Shrödinger simulations of laser-atom interaction would be impossible to couple with 3D propagation simulations. For the reason of computational costs, the quantum model that can be introduced to propagation simulations must be one-dimensional at most [2]. A fair question here is how good can be 1D-Shrödinger equation to describe the response of the realistic medium to the high-intense femtosecond laser field [3].

In this work, we develop a one-dimensional quantum model of an atom that can be introduced into propagation equations. We select potential pit which reproduces the energy levels of xenon atom. The linear dispersion of the potential pit simulated by us is in reasonable agreement with the experimental data. Our model reproduces the multiphoton and tunnel regimes of Xe atom ionization. At the central wavelength of 214 nm (1400 THz) we have shown the resonance enhanced multiphoton ionization of Xe, observed in Ref. [4]. We accelerated our program code by a factor of 10 using GPU instead of CPU.

Model parameters and equations



$$i\frac{\partial\Psi}{\partial t} = -\frac{1}{2}\frac{\partial^2\Psi}{\partial x^2} + U(x)\Psi - \mathcal{E}(t)x\Psi$$

With electric field

$$\mathcal{E}(t) = \sqrt{I}\exp\left[-\left(\frac{t}{\tau}\right)^2\right]\sin(2\pi\nu t)$$

where τ = 5 fs

which had the intensity I in range from 0.01 to 100 TW/cm^2 and frequency ν in range from 300 to 2000 THz (wavelength from 1 μm to 150 nm)

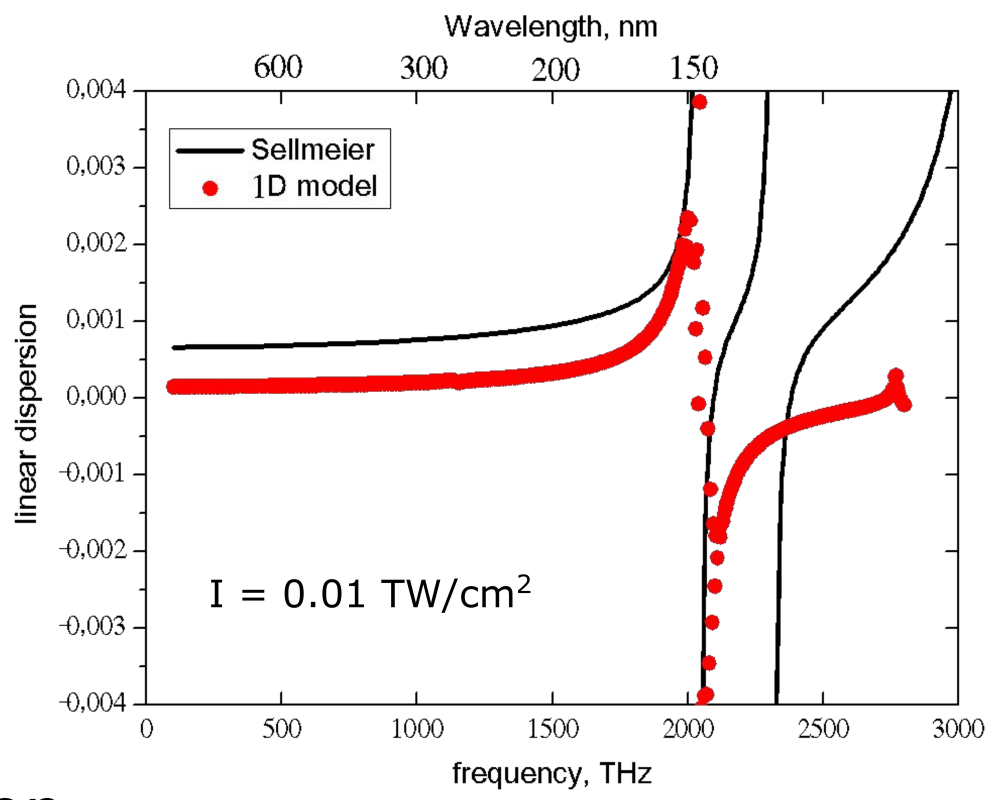
Lorentz pit with a super-gaussian cut-off:

$$U(x) = -\frac{0.5256}{\sqrt{x^2+0.63^2}}\exp\left[\left(-\frac{x}{8}\right)^{16}\right]$$

Three bound states with the energies of -12.08, -2.93 and -1.17 eV found using the stationary Shrödinger equation with potential $U(x)$.
The lowest two energies closely represent the ground and first exited ones of xenon atom with values -12.1 and -3.6 eV.

Linear dispersion

The linear dispersion evaluated for the intensities of 0.01–1 TW/cm^2 reproduced the Sellmeier-type dependence with the resonances corresponding to the ionization potential and excited levels.

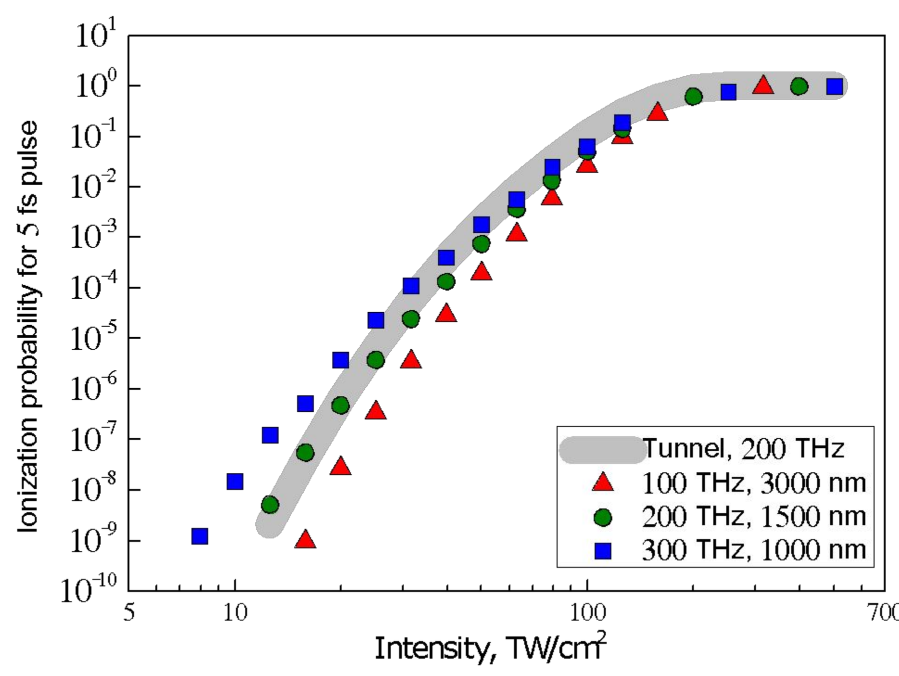


Tunnel and multiphoton ionization

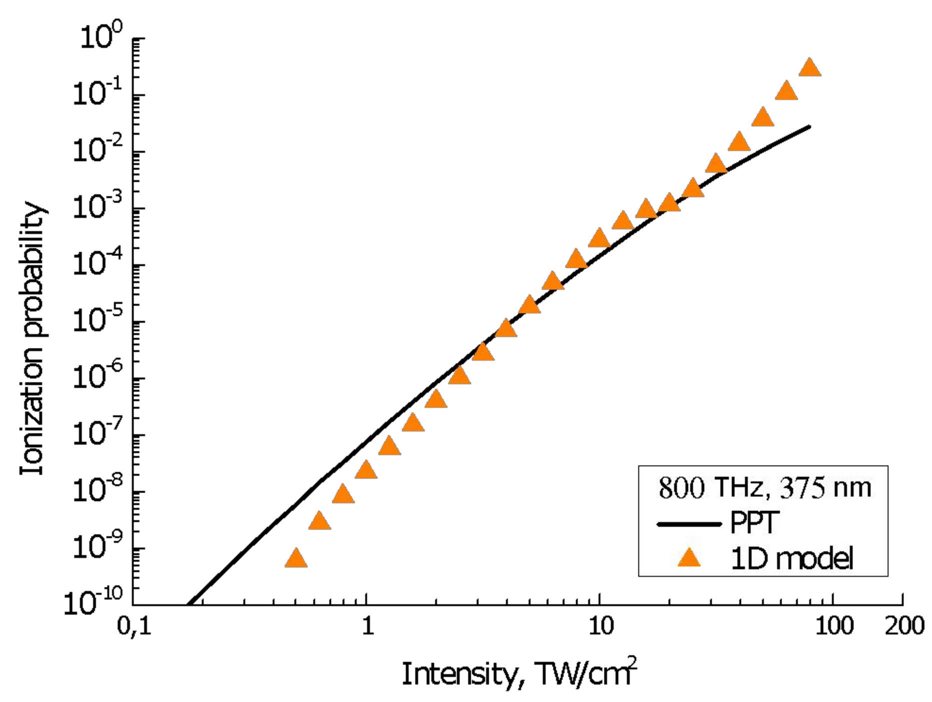
The tunneling ionization mechanism is used to describe the interaction of femtosecond infrared radiation with matter, and the ionization rate in this case is equal to

$$\mathrm{R}[E] = 4r_H^{5/2}\omega_{at}\frac{E_{at}}{E}\exp\left(-\frac{2}{3}r_H^{1/2}\frac{E_{at}}{E}\right)$$

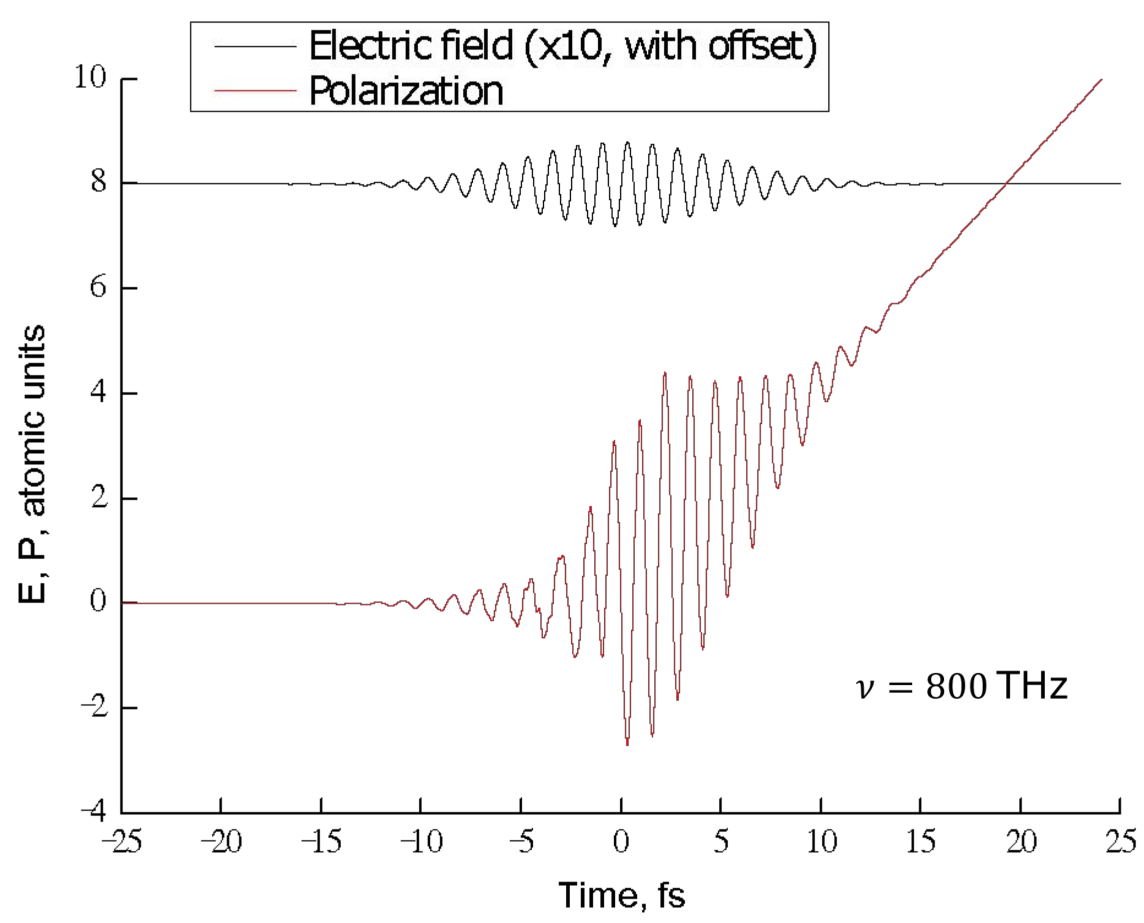
Tunnel ionization

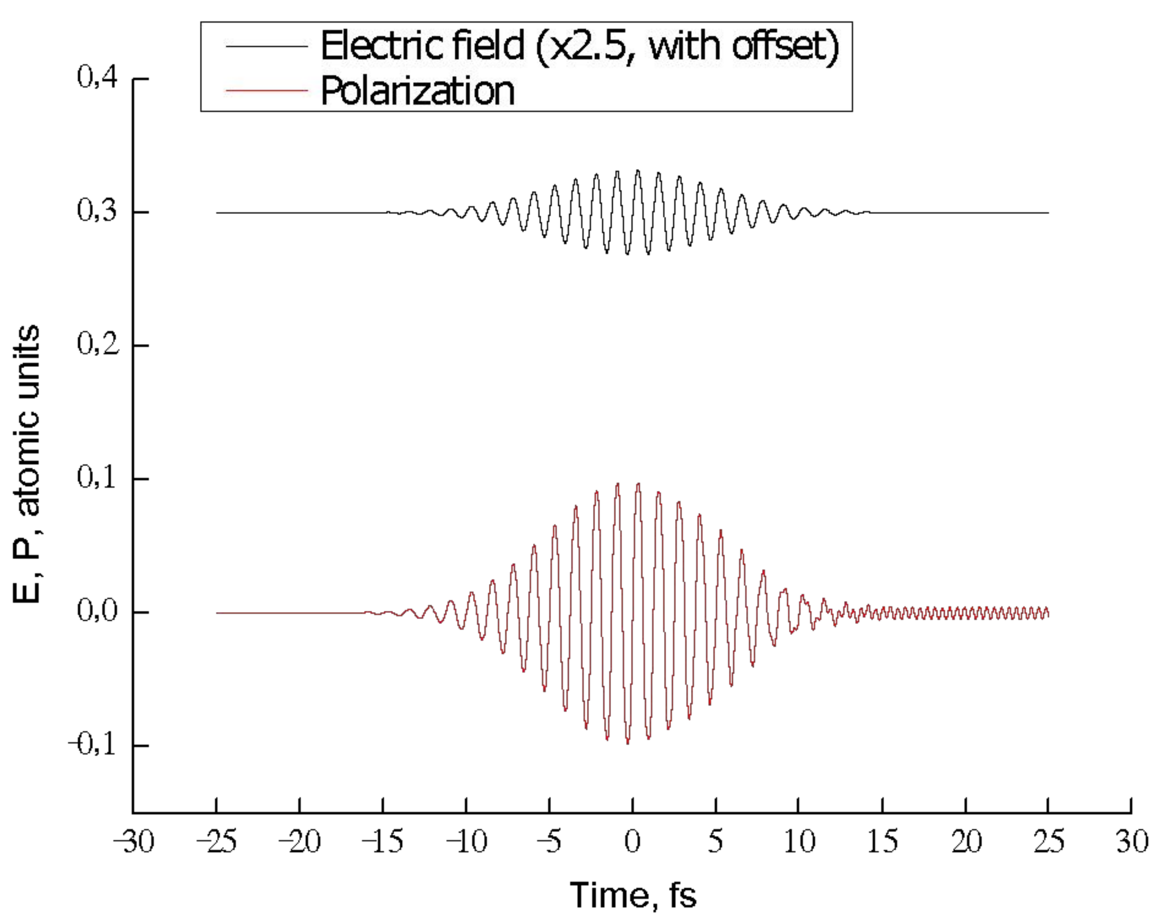


Multiphoton ionization

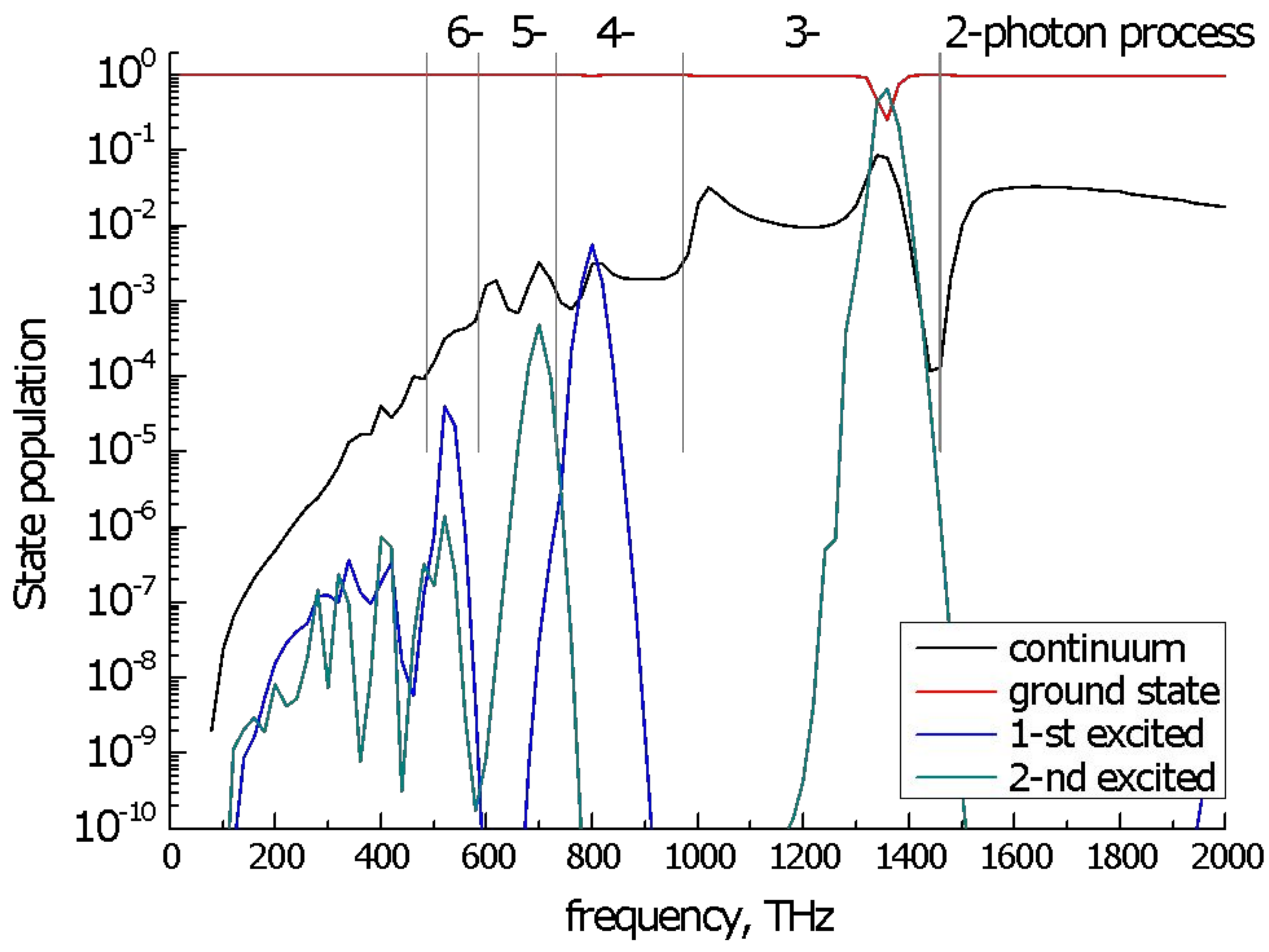


Nonlinear polarization

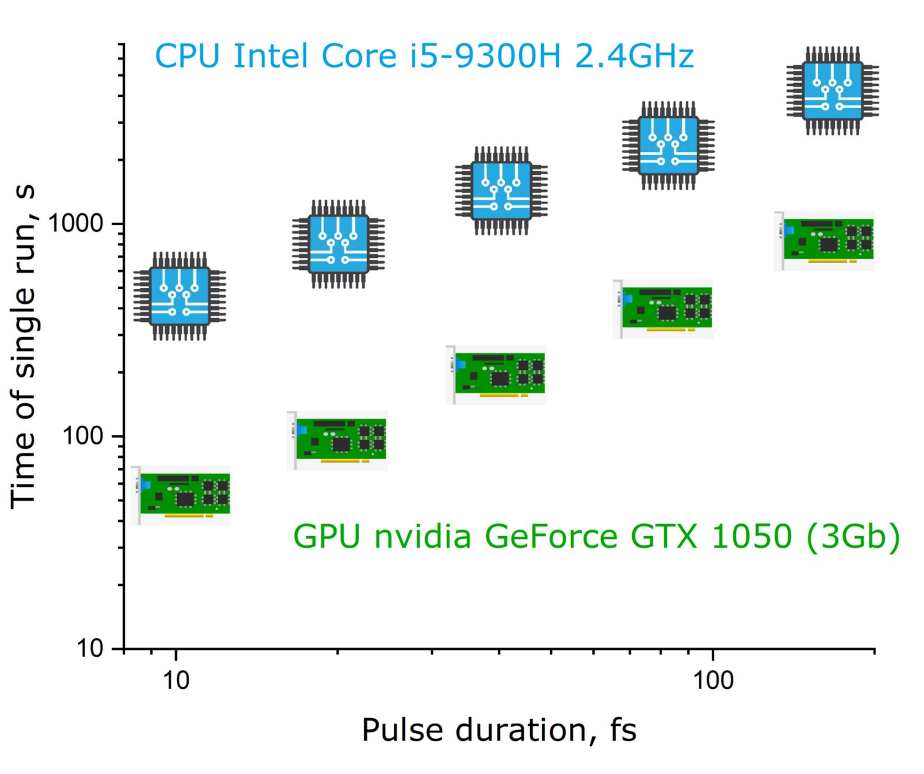




Resonance enhanced multiphoton ionization



GPU versus CPU



References

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