Boundary-free Scaling Calculations of Laser-Atom Interactions

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The most common approaches developed to describe laser-atom interactions are based on solving the time-dependent Schrödinger equation(TDSE) either directly on a numerical grid or in a basis set [1]. Neither approach allows the continuum electrons to escape beyond the boundaries, and reflections from these boundaries may result in unphysical interference. Although it is possible to enlarge the box or basis set at a given time step, or by introducing ad hoc absorbers near the boundaries, these approaches are inherently limited. Such limitations can be avoided, however, by adopting a scaled coordinate system, as shown recently by Sidky and Esry [2]. The scaled coordinate is chosen by rescaling the spatial coordinate according to $\xi = x/R(t)$, where $R(t)$ is set to approach γt at large time t, with γ being an arbitrary velocity. Thus, in the scaled coordinate, the electron position does not expand with time.

Figure 1. Free propagation of a Gaussian wave packet.

As an illustration, in Fig. 1 we show the free propagation of a Gaussian wavepacket. The velocity and width of the wavepacket are both 1 a.u. at $t = 0$. The real part of the wavefunction at $t = 10$ and $t = 20$ is plotted. The solid lines are for the scaled wavefunction and the dotted lines are for the weighted physical function $\sqrt{R}\Psi(R\xi, t)$. The abscissa is the scaled coordinate ξ, with the scaling paramter $R(t) = \sqrt{1 + t^2}$ for $t \geq 0$. At large time, the scaled wave function is time independent and is given by

$$\Phi(\xi) = [\frac{a^2\gamma^2}{2\pi}]^{\frac{1}{4}} \exp\,[-\frac{1}{4}a^2\gamma^2(\xi - \frac{v_0}{\gamma})^2] \qquad (1)$$

where a and v_0 are the initial width and velocity, respectively. In this example the center of the wavepacket is located at ξ=1.0 in the scaled coordinate ξ, but the spread of the wavepacket in the real space is large, and the oscillation of $\Psi(R\xi, t)$ is rapid. In the scaled space, on the other hand, the wavefunction is smooth. Examples using scaled coordinates for atoms in an intense laser field will be shown. In addition, in the scaled coordinates the probability density also contains information on the ATI peaks directly, Fig. 2. Here we show how the ATI peaks match the peaks of the density of the wavefunction at the asymptotic time in the scaled space. Details of these calculations will be presented at the conference.

Figure 2. ATI spectrum (dashed line) and density plot (solid line). The horizontal axis is the scaled coordinate (or the velocity of electron divided by scaling contant γ).

Acknowledgments: This work is supported by the Chemical Sciences,Geosciences and Biosciences Division, Office of Basic Energy Sciences, Office of Science, U. S. Department of Energy.

References

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