Computational Physics Final Project

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1 Solving the Time-Dependent Schrödinger Equation

1.1 Setup

To solve the time-dependent Schrödinger equation for a hydrogen atom in a modified "soft-core" Coulomb potential exposed to a strong laser, we are using the leapfrog method. To start the leapfrog method, we need our initial wavefunction and the wavefunction after one time-step. We re-used our program from Project 8, specifically from the Coulomb potential portion of the project, in order to produce the initial wavefunction. The second time-step is calculated in free space, meaning it can represented by $\Psi_1(x) = \Psi_0 e^{-iE_i dt}$, where E_i is the first energy from figure 2 (-0.6698596).

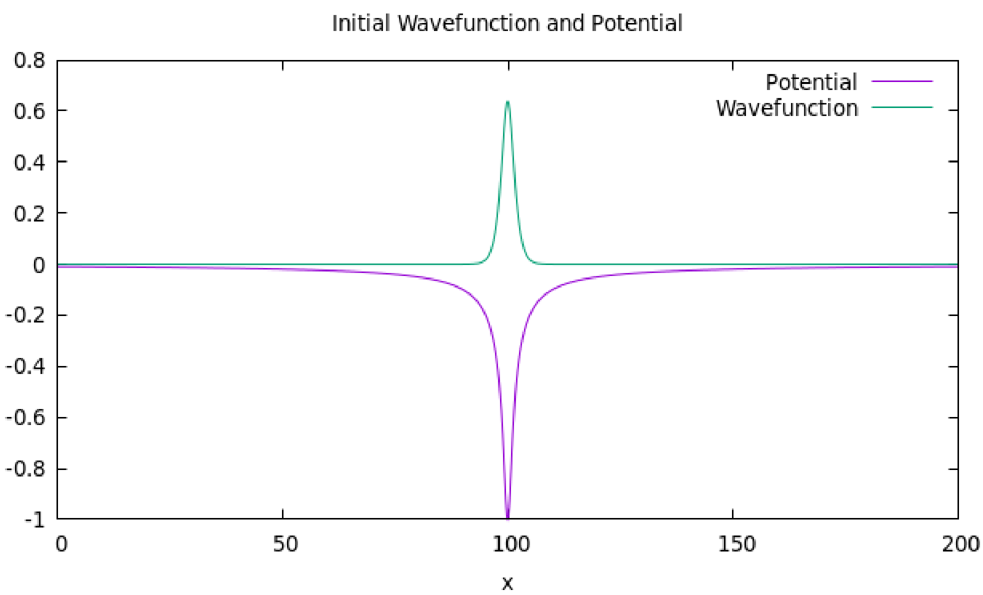

Figure 1: Ψ_0 and V

Note that 2,000 points and a spatial step of 0.1 were used to produce the initial wavefunction and potential used in this project. Also, note that the energies in figure 2 are similar to that in Table 1 of Javanainen *et al.* [1]

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energies for l =   0:
 -6.698596E-01 -2.749824E-01 -1.515176E-01 -9.271876E-02 -6.355224E-02 -4.550619E-02 -3.461178E-02 -2.689517E-02 -2.171151E-02 -1.773153E-02
```

Figure 2: Energy eigenvalues for initial wavefunction

The electric field acting on the atom was created by applying an envelope of $\sin^2(\pi t/T)$, making the total electric field $E(t) = E_0 \sin^2(\pi t/T)\sin(\omega t)$, where $E_0 = 0.1$, $\omega = 0.148$ and $T = 1200.0$.

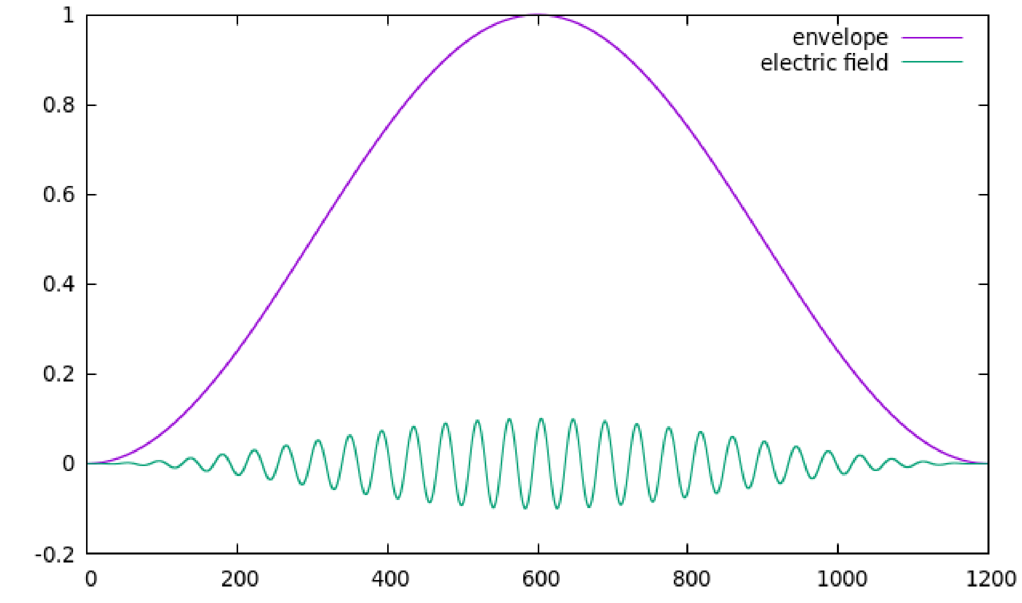

Figure 3: Envelope and electric field

1.2 Propagation

After the second time-step, the wavefunction is propagated via the leapfrog method. The total time of the laser pulse was 1,200, which matches that of the electric field. The largest time-step allowing us to get a stable norm and accurate survival probability was 0.00455. The time this program took to run was about 12.8 seconds when wavefunctions weren't written to output.

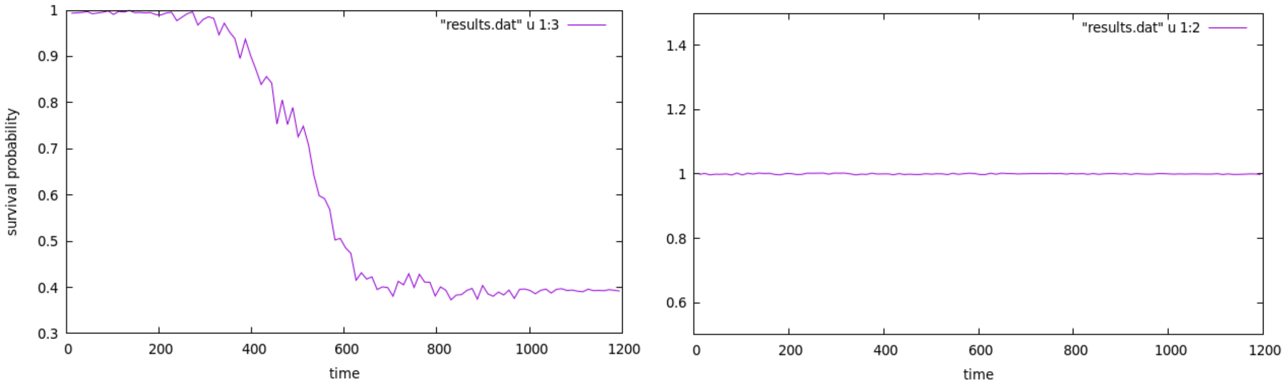

Figure 4: Survival probability and norm of a time-step of 0.00455

1.3 Impact of changing the spacial step

The last thing we investigated was the impact of cutting our spacial step h in half, from 0.1 to 0.05. As predicted, the size of the time-step needed for convergence is a fourth of what it was when $h = 0.1$.

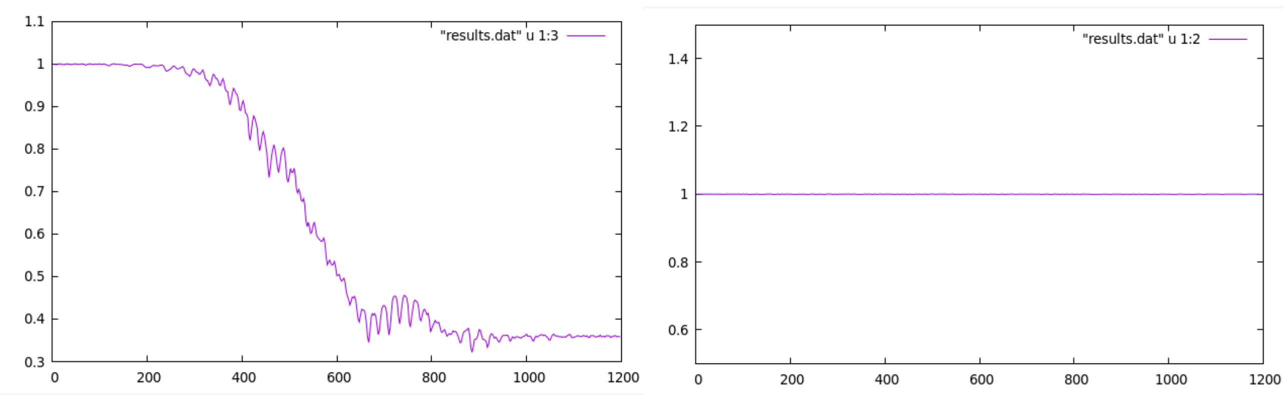

Figure 5: Survival probability and norm of $h = 0.05$ with time-step of 0.001

References

[1] J. Javanainen, J.H. Eberly, and Qichang Su, Phys. Rev A **38** (1988) 3430.