Electron Trajectory

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Generating trajectories

After reading through the Thomas Siegel thesis a couple of times, I came to grips first with the intuitive side of the three step model, and later the mathematics. Afterwards, my task was to program the trajectory of the electron after it leaves the atomic potential, initially I tried to do this with seaborne, in order to learn a new skill and make some pretty graphs, but eventually realized it wasn't as well suited to the types of plots I wanted to make as good old matplotlib, so I settled for that instead. After a couple of attempts at inserting the formula found in the thesis:

$$x(t) = \frac{-e}{m\omega_0^2}\left[E_0(t)cos(\omega_0 t + \phi) - E_0(t_i)cos(w_0 t_i + \phi)\right] - \frac{-eE_0(t_i}{m\omega_0^2}(t - t_i)sin(\omega_0 t + \phi) \tag{1}$$

After some attempting and tinkering, I did not manage to implement the formula, and still have a couple of doubts as to the terms, so instead I used the traditional equations of motion, which yielded much better results:

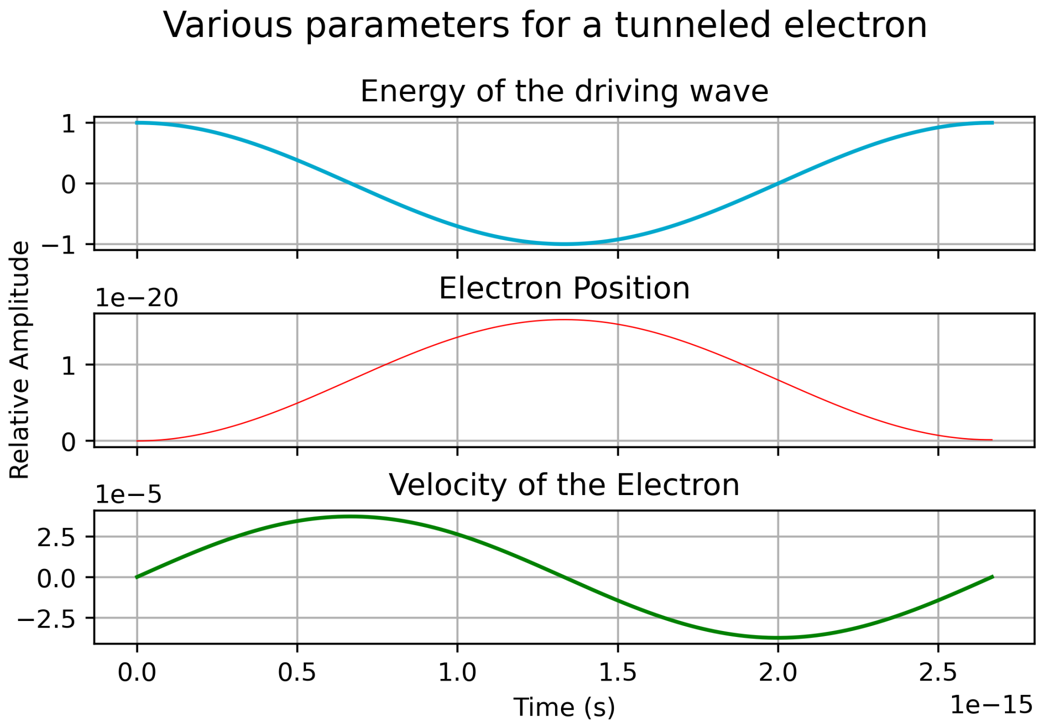

Figure 1: Pretty (and) self explanatory graph

Satisfied with this graph, which accurately (I think) describes the motion of the electron and the velocity. I also created a github repository to keep track of the code (and for postgrad/employers of course) which is linked here: https://github.com/alex-benitez/Atto

Additionally you can add phase to the trajectory, and get a slightly different graph:

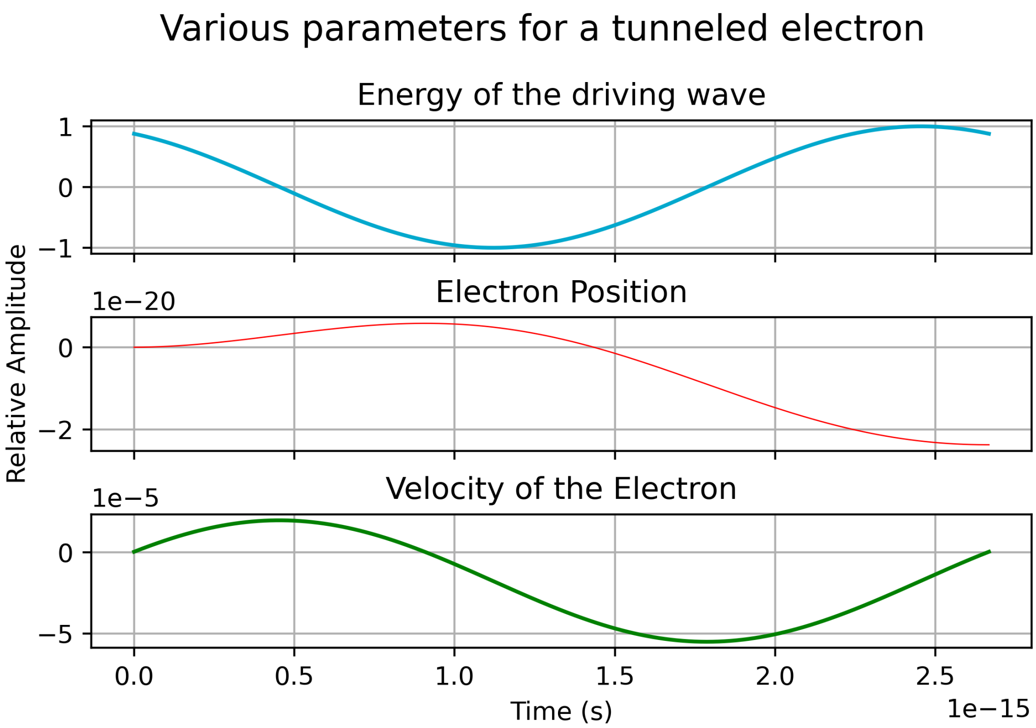

Figure 2: Added phase of 0.5 radians

The next logical step is to create a distribution of electrons exiting the nucleus at a given phase, and use that to plot the graph of possible positions.

After tweaking the colours around to make the graph more readable, I arrived at the following plot, this is very close to the plot found in the thomas siegel thesis which as a good sign.

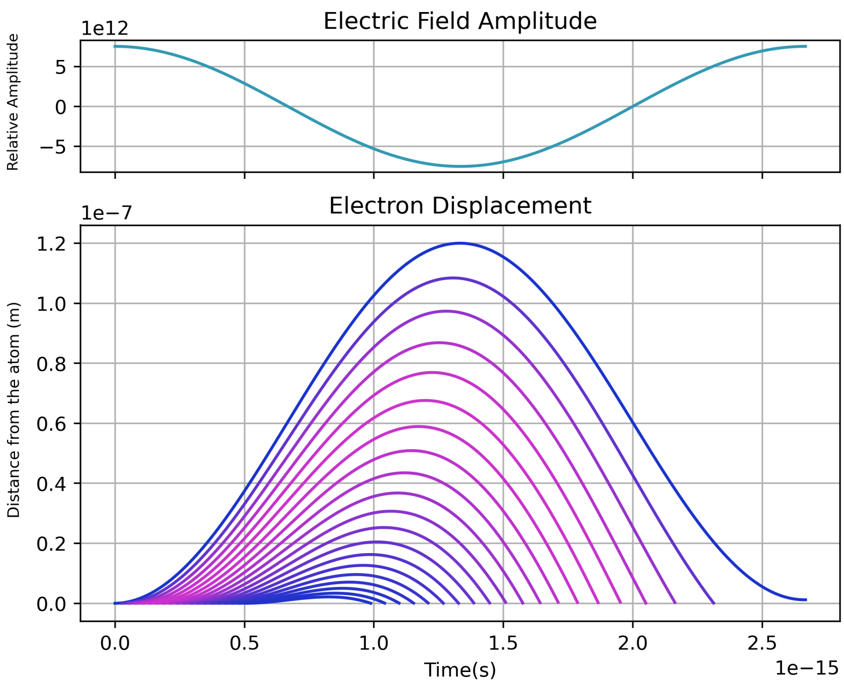

Figure 3: Electron displacement as a function of initial phase to the electric field (more purple values have higher peak kinetic energy)

The next logical step of course was to plot the kinetic energy with respect to phase. After some extra calculations and making the code far more efficient (unnecessary but I learnt quite a bit of numpy along the way).

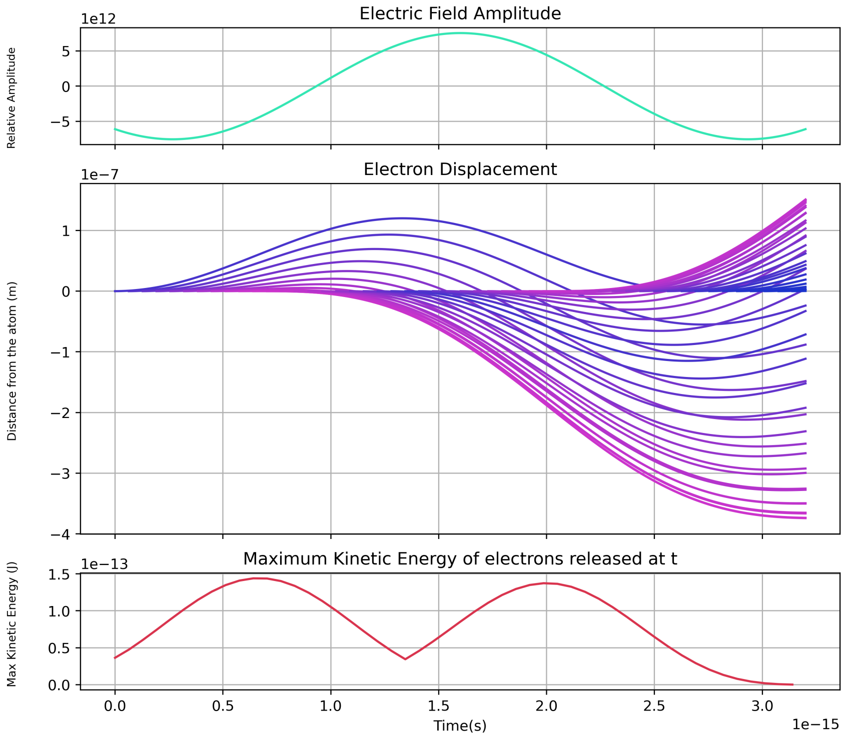

Figure 4: Kinetic Energy of the electron as a function of initial phase with respect to an electric field

I should probably change the colour scheme becaus it looks pretty but isn't as clear as other similar graphs; I'll ask Ben how he did it.