Computational Physics: PS 10

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1 Discussion

My GitHub repo is `https://github.com/marcusHoskinsNYU/phys-ga2000`. For images that are blurry here, please see the ps-10 folder for individual image files.

1.1 Problem 1

1.1.1 Part (a)

The relevant code is given in the repo.

1.1.2 Part (b)

The relevant code is in the repo. In lieu of providing an actual animation, here we have provided several snapshots from the time evolution of our initial wavefunction. These are seen in figures 1, 2, 3, and 4. A more complete set of such images are found in the repo.

1.1.3 Part (c)

After running the animation for a while, we see that the initially localized electron wavefunction begins to "bounce back and forth between the walls of the container" in classical terms. What is happening quantumly, of course, is that the wavefunction is moving left/right due to time evolution. And, at each wall the wavefunction obeys a certain set of reflection conditions, which here are such that no part of the wavefunction is transmitted through the wall. Over time, the initially localized wavefunction begins to become less localized. This occurs because of the uncertainty principle.

At some later time $t = 1.00 \times 10^{-13}$s, we see in figure 5 that the electron wavefunction is noticeably less local than when it began in figure 1.

1.2 Problem 2

1.2.1 Part (a)

The relevant code is given in the repo.

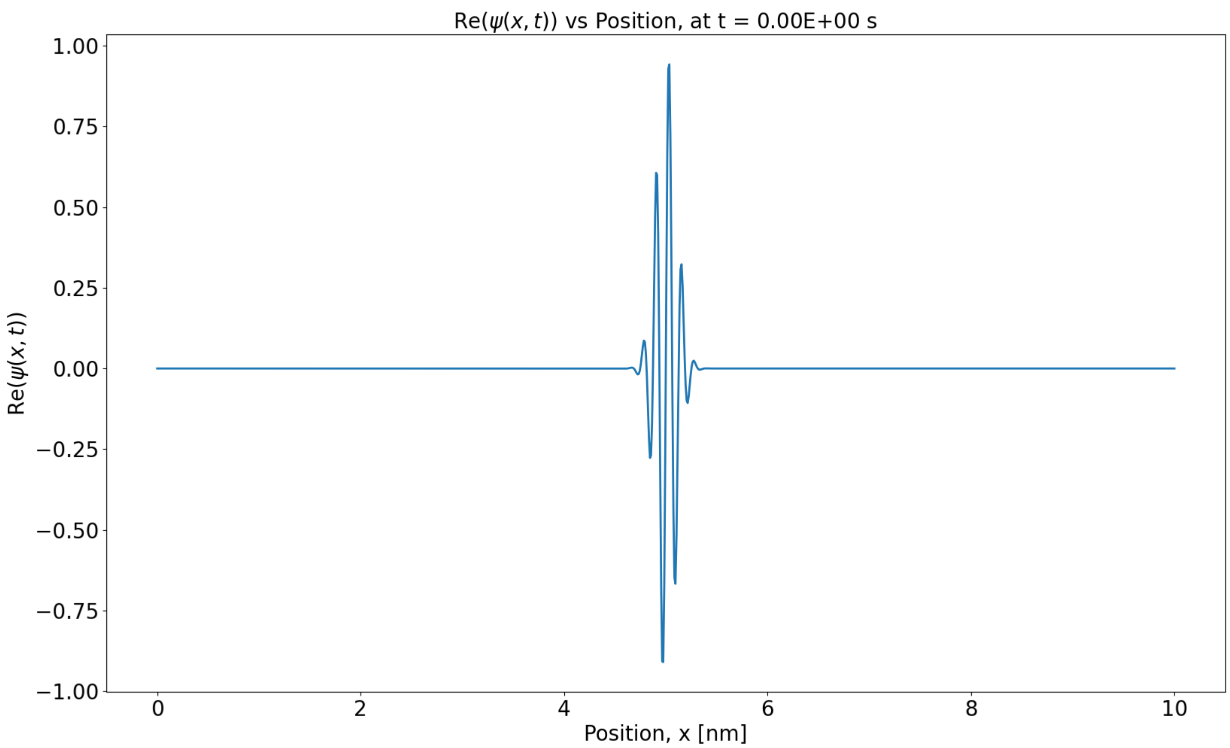

Figure 1: This is our electron's initial wavefunction, before any time evolution has occurred.

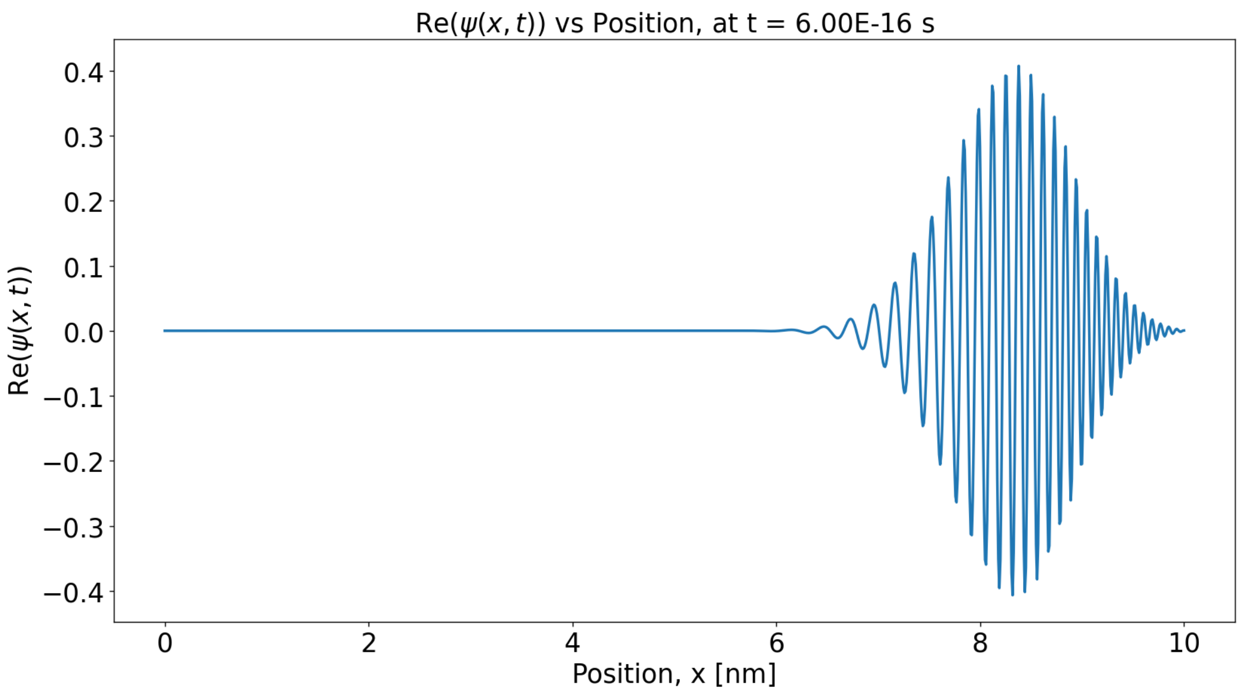

Figure 2: This is $t = 6.00 \times 10^{-16}$s after $t = 0$ for our electron. We see that it is moving towards the right wall. We have numerically evolved in time using the Crank-Nicolson method.

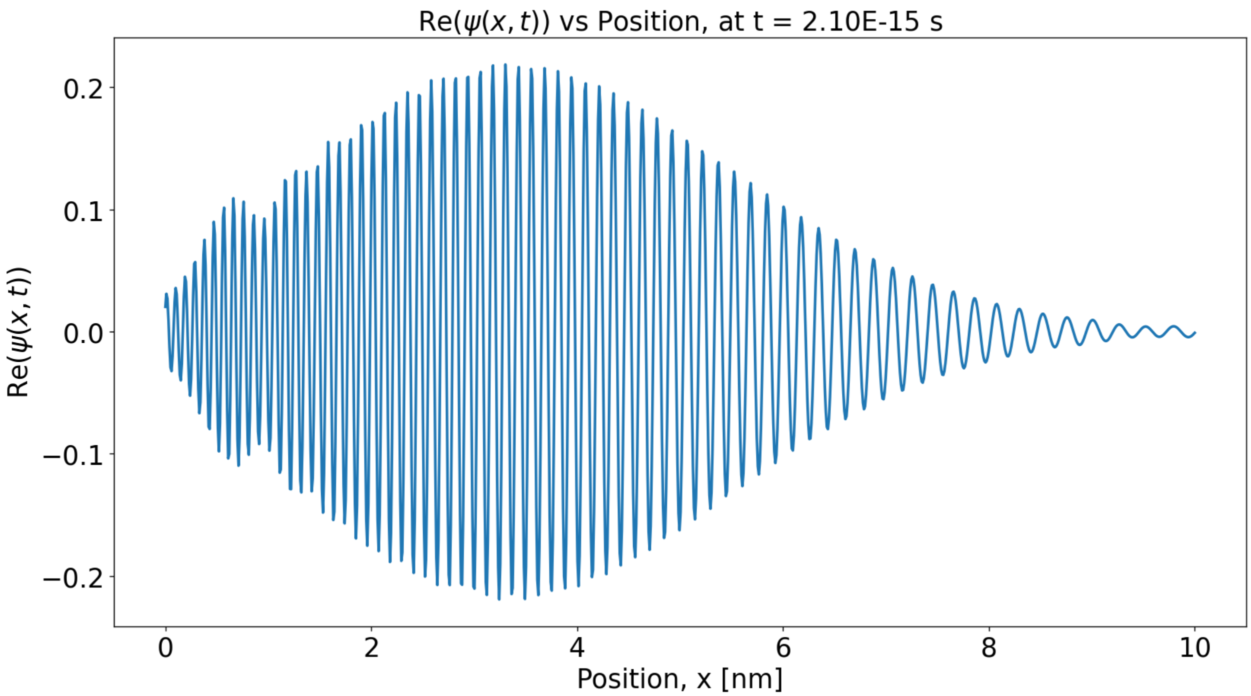

Figure 3: This is $t = 2.10 \times 10^{-15}$s after $t = 0$ for our electron. We see that it has "bounced off the right wall", in classical terms, and is moving towards the left wall. We have numerically evolved in time using the Crank-Nicolson method.

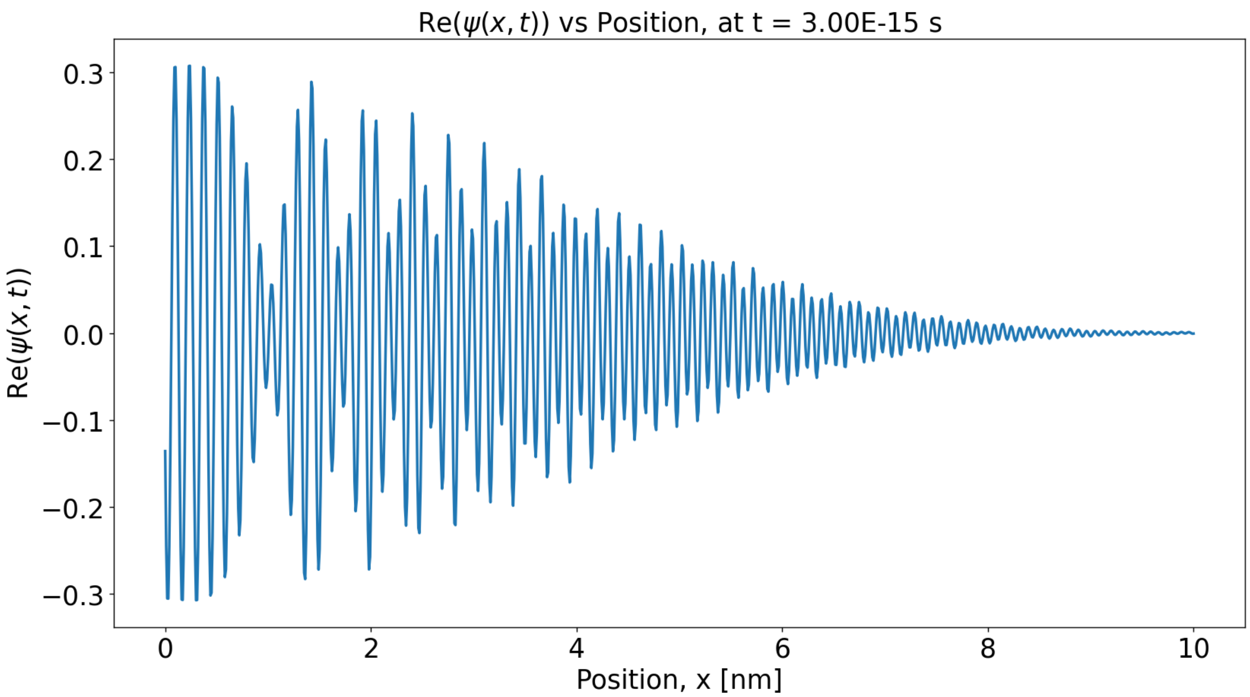

Figure 4: This is $t = 3.00 \times 10^{-15}$s after $t = 0$ for our electron. We see that it has "bounced off the left wall", in classical terms, and is moving back towards the right wall. Notice that the wavefunction is getting less localized and is getting "messier", or more nonlocal. We have numerically evolved in time using the Crank-Nicolson method.

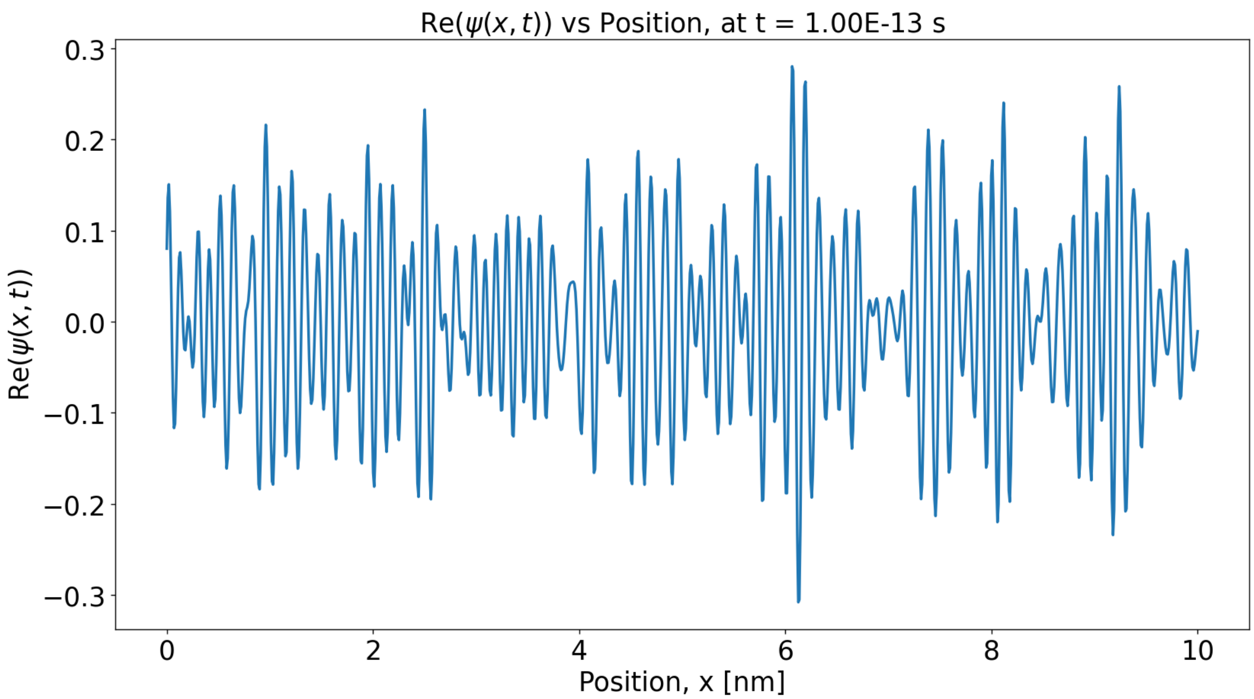

Figure 5: This is $t = 1.00 \times 10^{-13}$s after $t = 0$ for our electron. We see that it is far less local than when it began (c.f. figure 1). We have numerically evolved in time using the Crank-Nicolson method.

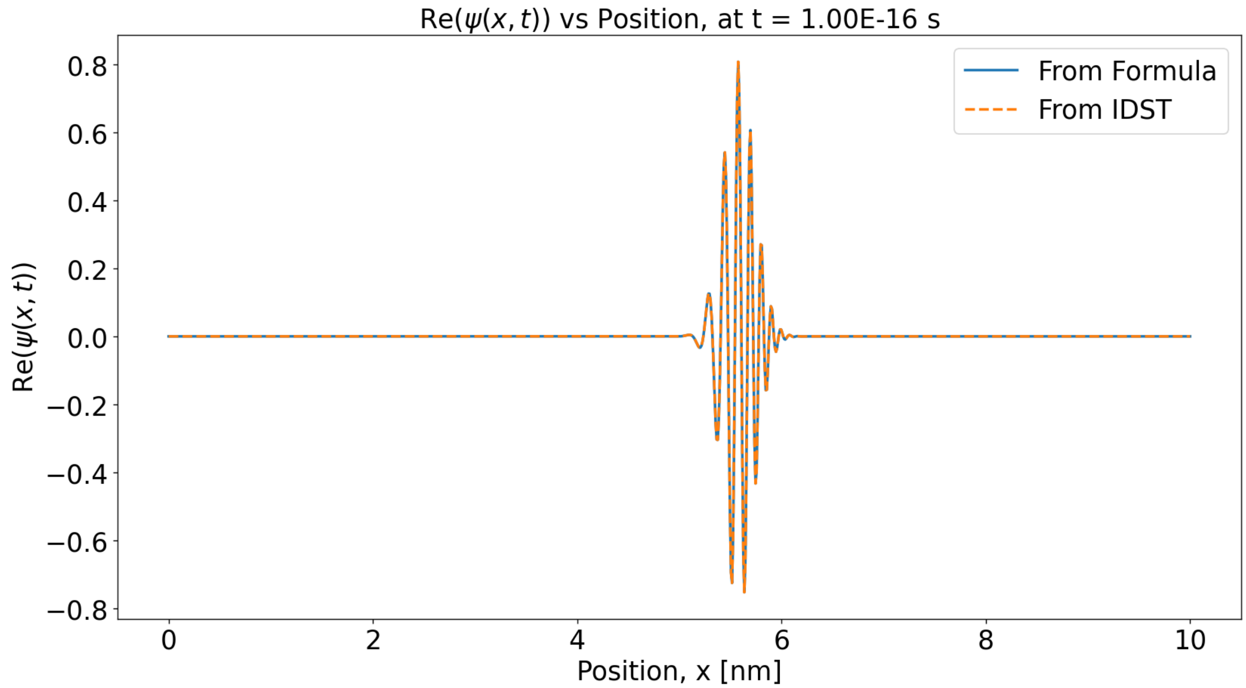

Figure 6: In this plot, we compare the real part of the electron's wavefunction at some later time (time evolved using the spectral method). The blue plot is constructed using the given formula, and the orange dashed plot is constructed using an inverse discrete sine transform. As we can see, these two methods agree.

1.2.2 Part (b)

The relevant code is given in the repo. The comparison of the two ways of obtaining the relevant wavefunction is seen in figure 6. As we can see, the two methods agree.

1.2.3 Part (c)

The relevant code is in the repo. In lieu of providing an actual animation, here we have provided several snapshots from the time evolution of our initial wavefunction. These are seen in figures 7, 8, 9, and 10. A more complete set of such images are found in the repo. Notice how these look very similar to the corresponding plots tiem evolved using the Crank-Nicolson method, figures 1, 2, 3, and 4.

1.2.4 Part (d)

After running the animation for a while, we see that the initially localized electron wavefunction begins to "bounce back and forth between the walls of the container" in classical terms. What is happening quantumly, of course, is that the wavefunction is moving left/right due to time evolution.

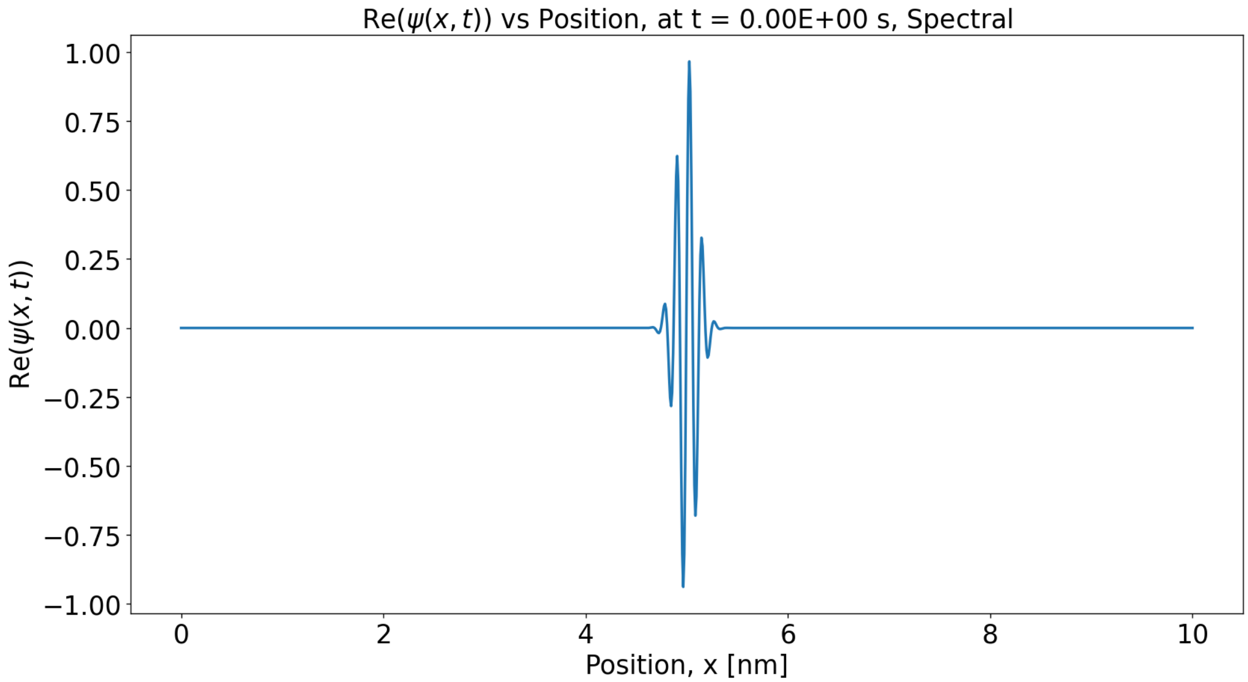

Figure 7: This is our electron's initial wavefunction, before any time evolution has occurred.

And, at each wall the wavefunction obeys a certain set of reflection conditions, which here are such that no part of the wavefunction is transmitted through the wall. Over time, the initially localized wavefunction begins to become less localized. This occurs because of the uncertainty principle.

At some later time $t = 1.00 \times 10^{-11}$s, we see in figure 11 that the electron wavefunction is noticeably less local than when it began in figure 7. We also notice an interesting form of the wavefunction, occurring at time $t = 1.00 \times 10^{-13}$s and seen in figure 12. While the wavefunction here is still not as local as where it began, there is interesting structure.

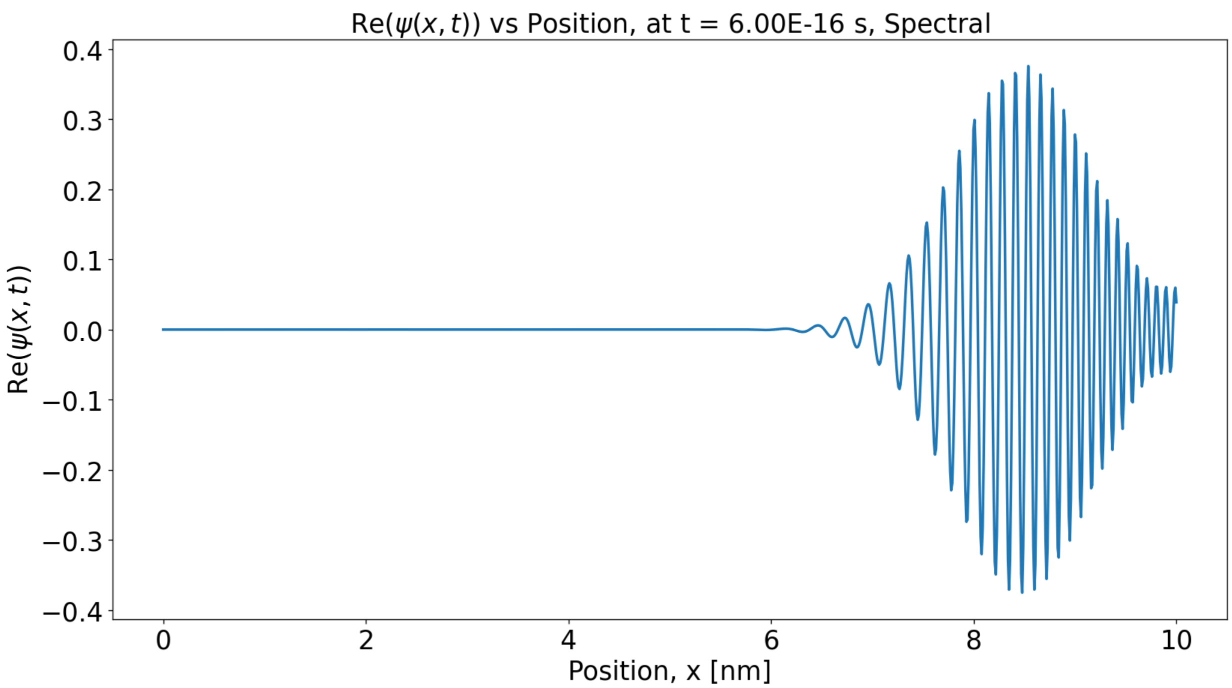

Figure 8: This is $t = 6.00 \times 10^{-16}$s after $t = 0$ for our electron. We see that it is moving towards the right wall. Note how similar this looks to figure 2. We have numerically evolved in time using the spectral method.

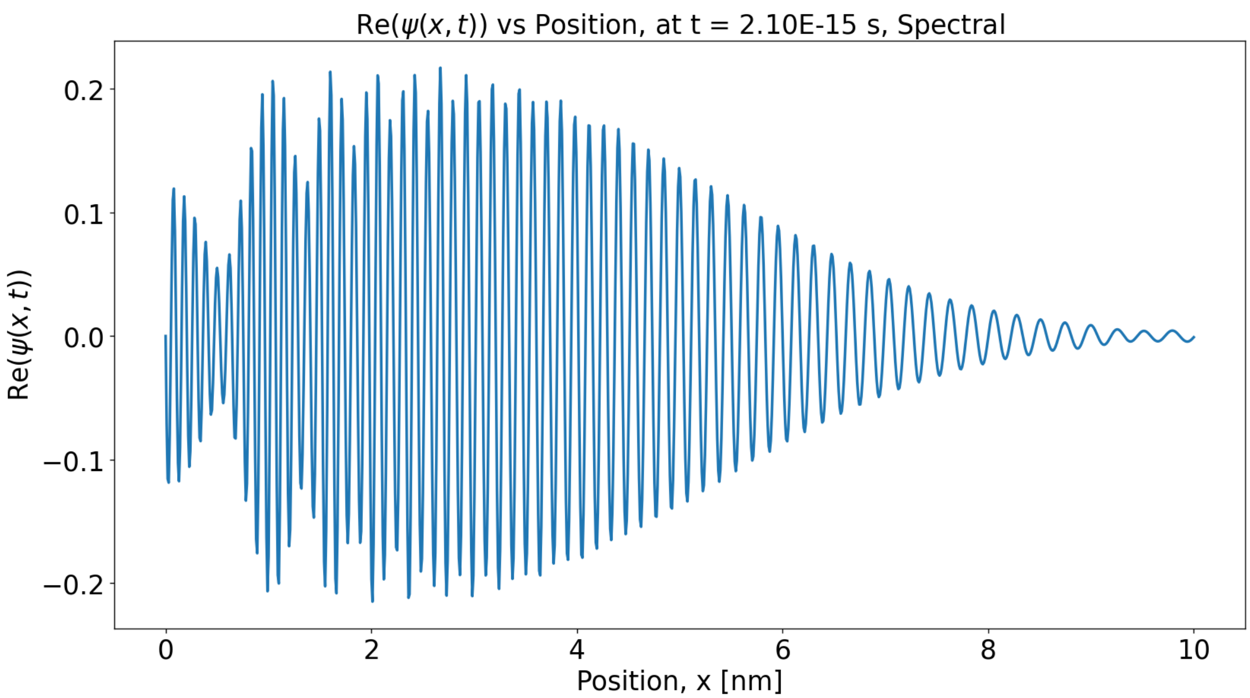

Figure 9: This is $t = 2.10 \times 10^{-15}$s after $t = 0$ for our electron. We see that it has "bounced off the right wall", in classical terms, and is moving towards the left wall. Note how similar this looks to figure 3. We have numerically evolved in time using the spectral method.

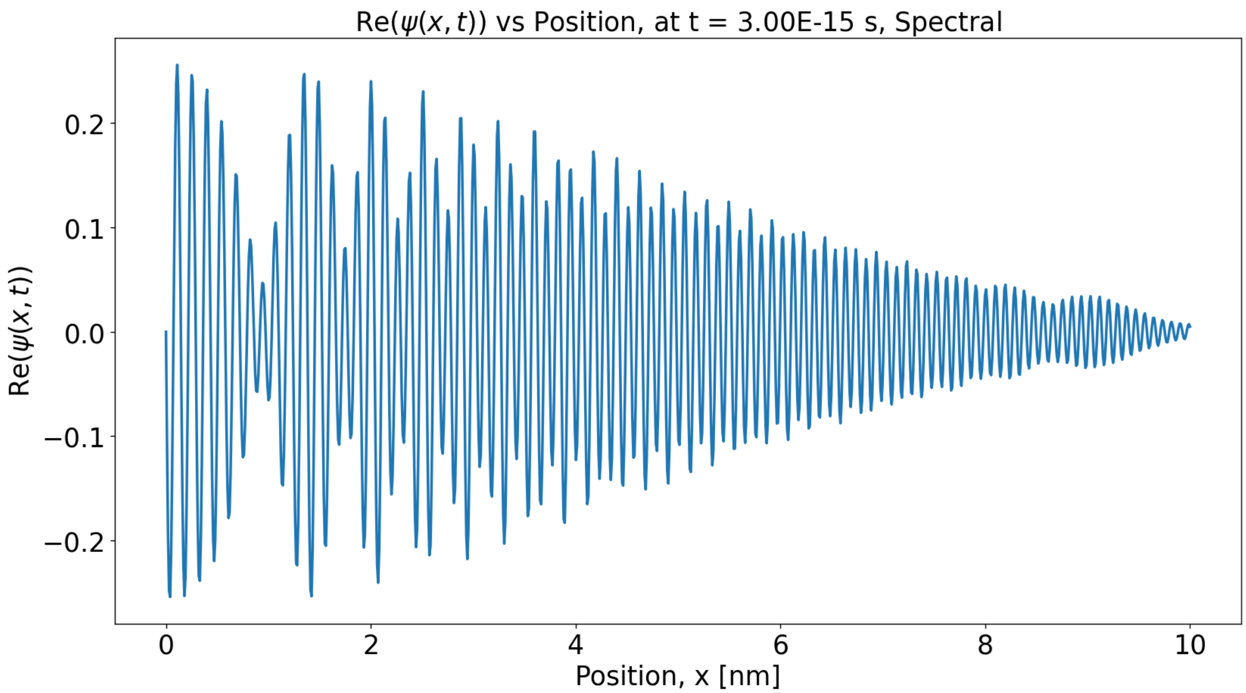

Figure 10: This is $t = 3.00 \times 10^{-15}$s after $t = 0$ for our electron. We see that it has ”bounced off the left wall”, in classical terms, and is moving back towards the right wall. Notice that the wavefunction is getting less localized and is getting ”messier”, or more nonlocal. Note how similar this looks to figure 4. We have numerically evolved in time using the spectral method.

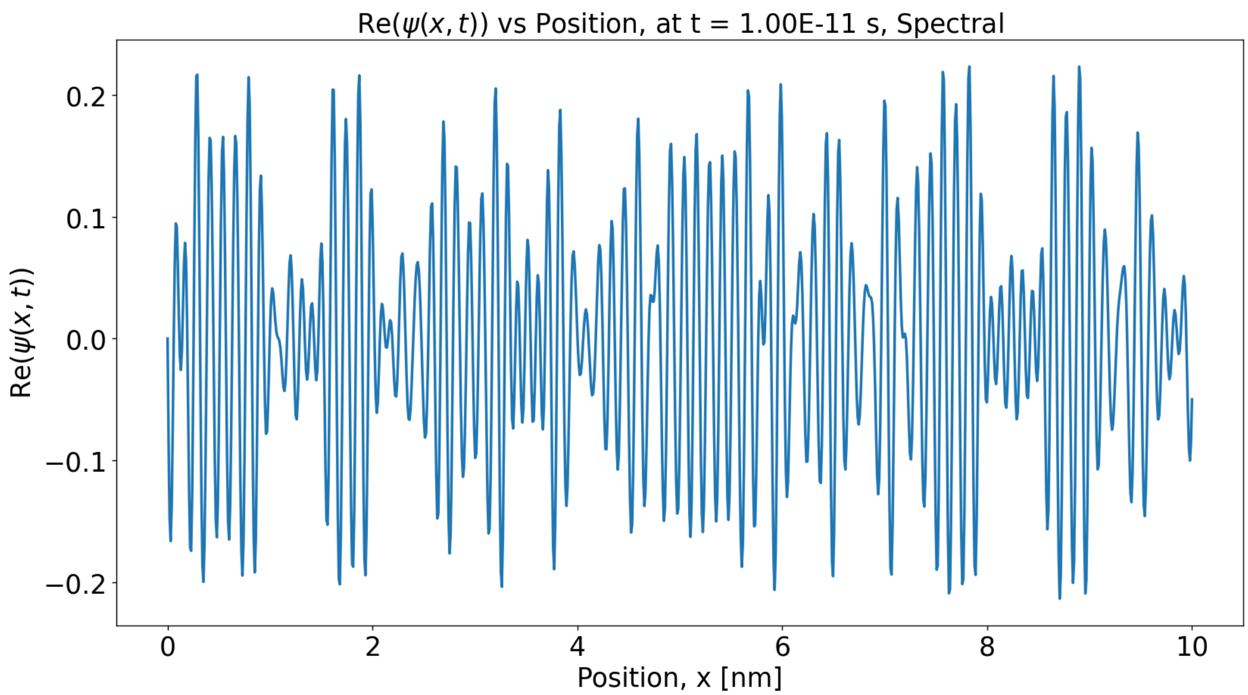

Figure 11: This is $t = 1.00 \times 10^{-11}$s after $t = 0$ for our electron. We see that it is far less local than when it began (c.f. figure 7). We have numerically evolved in time using the spectral method.

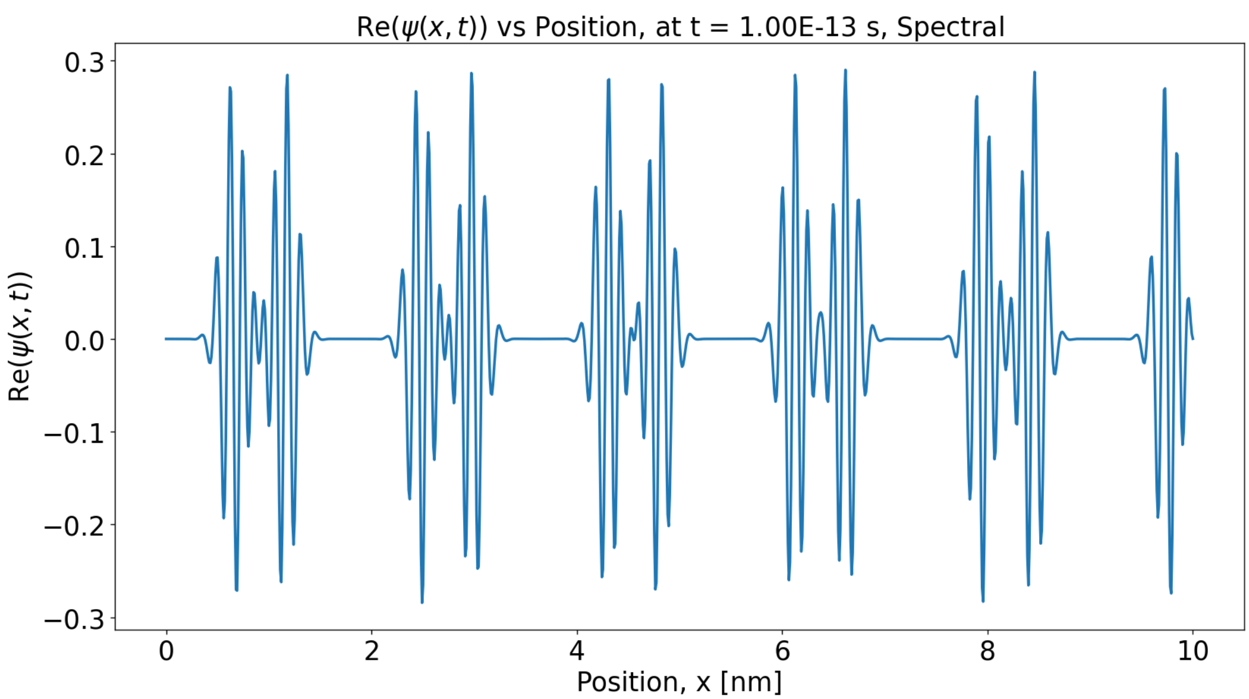

Figure 12: This is $t = 1.00 \times 10^{-13}$s after $t = 0$ for our electron. We see that, while it is far less local than when it began (c.f. figure 7), there is interesting structure in the wavefunction. We have numerically evolved in time using the spectral method.