

# **Lab # 1**

## **Travelling Wave-packets**

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## 1. Matter Wavepackets based on Fourier Series

1(a)

$$\text{Average Wavelength } (\lambda_o) = h/p_o = h/\sqrt{e * E_o * 2 * m} = 3.5426\text{e-10 (m)} = 0.35426 \text{ (nm)}$$

$$\text{Energy} = \sqrt{e * E_o * 2 * m} = 1.8704\text{e-24 (kg}\cdot\text{m/s)}$$

$$\text{Phase Velocity } v = h * k / 2m = h * \pi / 2 * \lambda_o * m = 6.626\text{e-34} * \pi / 0.35426 * 2 * 9.1094\text{e-31} = 3.222\text{e6 (m/s)}$$

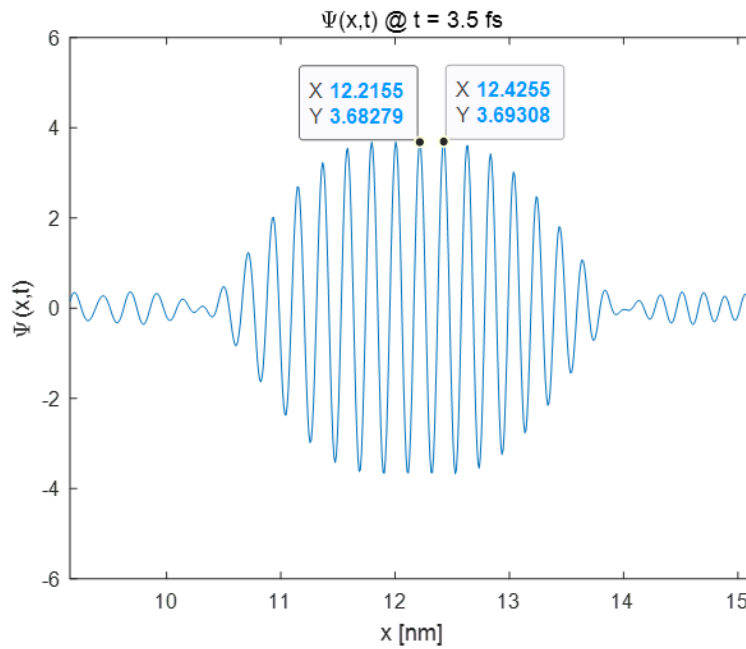
$$\text{Group Velocity } v = h * k / m = 6.444\text{e6 (m/s)}$$

1(b)

$$C_n = A = [0.1 \ 0.2 \ 0.3 \ 0.4 \ 1 \ 1.4 \ 1 \ 0.4 \ 0.3 \ 0.2 \ 0.1];$$

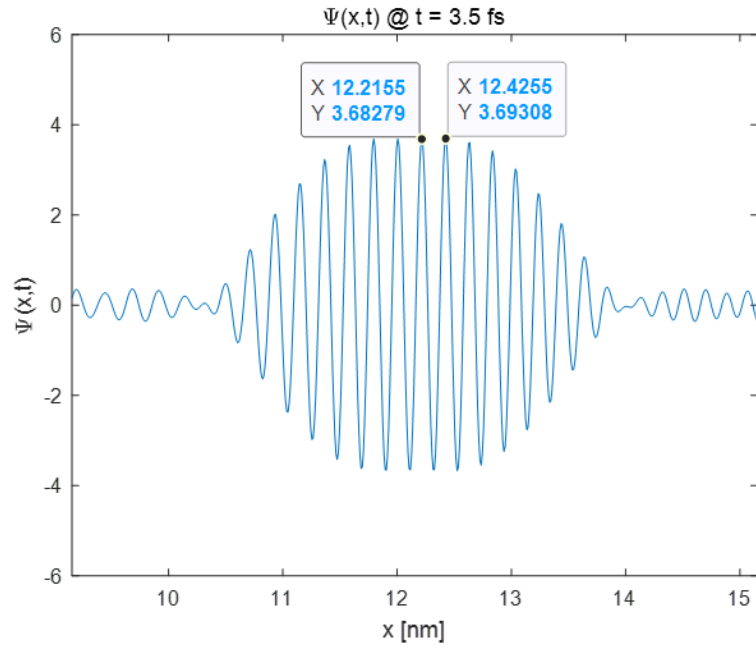
$k$  is in the range of  $k = 25:35$ ,  $k_{avg} = \text{mean}(k) = 30$

1(c)



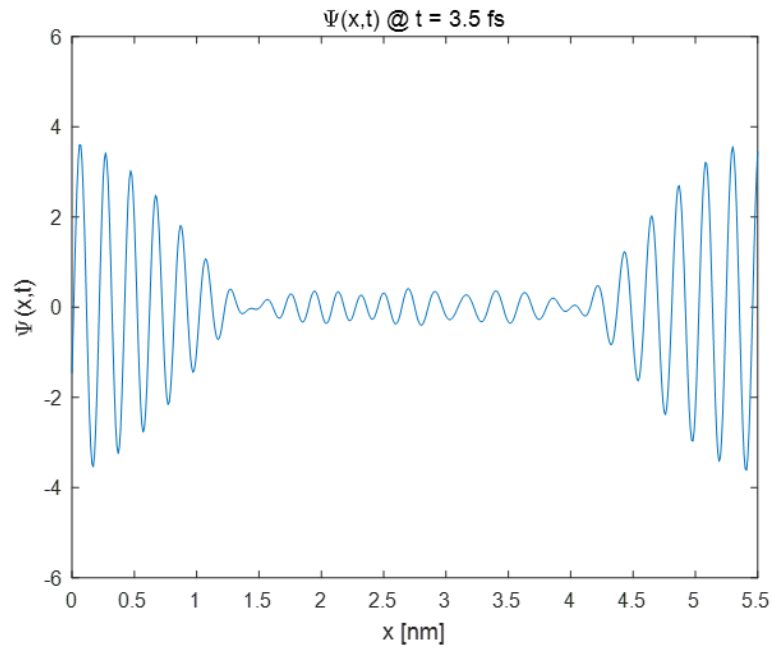
By the distance between two adjacent waveform peaks  $\Delta x_{\min} = 12.4255 - 12.2155 = 0.21$ ,  $\Delta k = (35 - 25)/5.5 = 1.818$ .

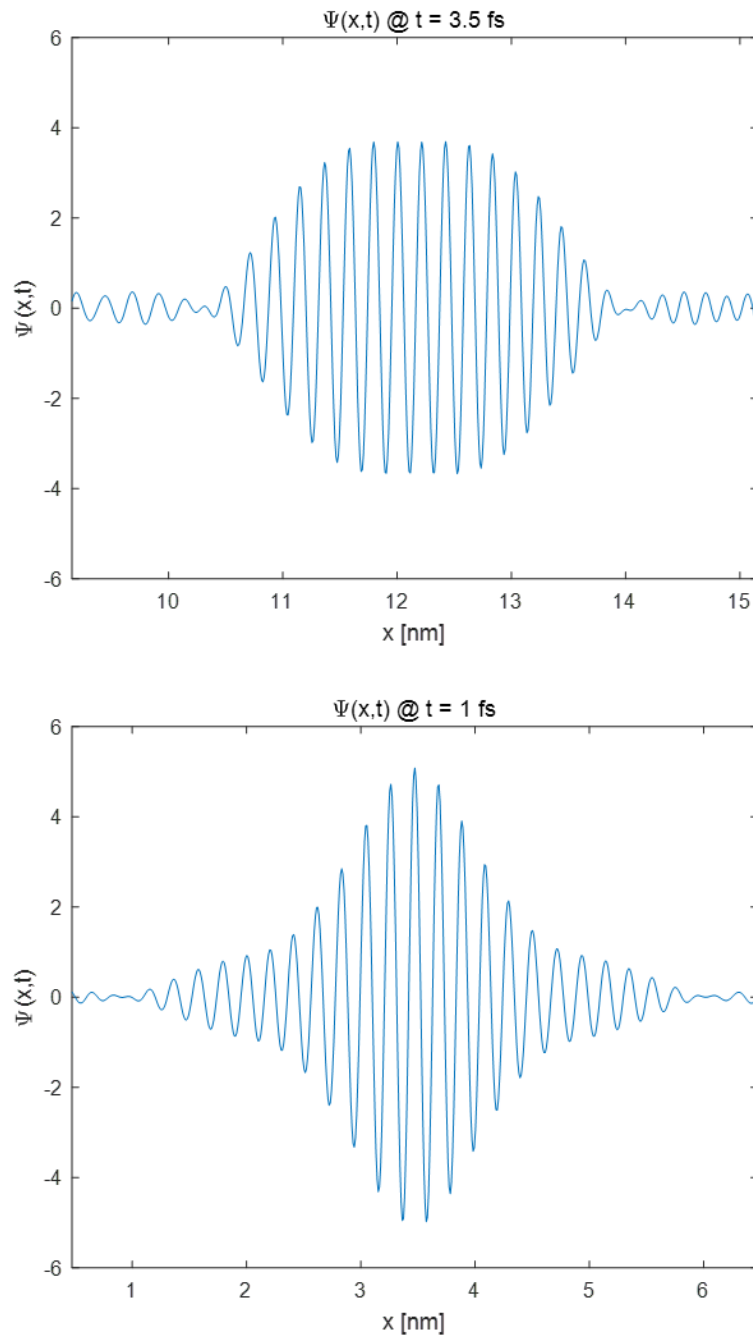
1(d)



Simulation waveform results in  $\Delta x = 0.21$  (nm)

1(e)



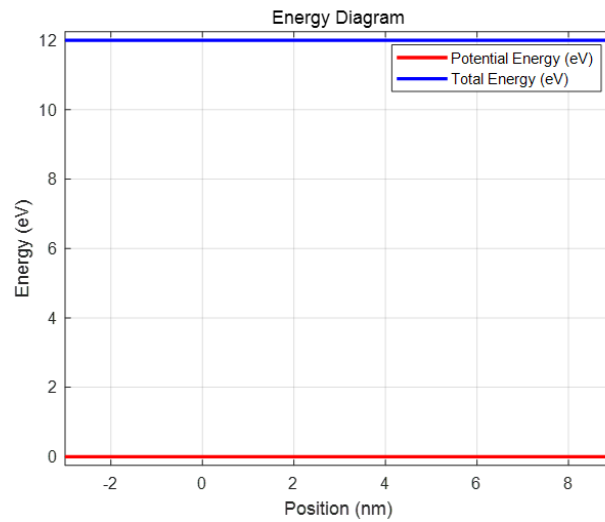


It can be seen from the waveform diagram of 1fs that the phase velocity is approximately 3.5, this corresponds closely to the calculated phase velocity  $v = 3.222 \text{ (nm/fs)}$ .

## 2.Traveling Gaussian Wave packet in Force-Free Space

FLAG\_plot\_Energy\_Diagram(line 24)

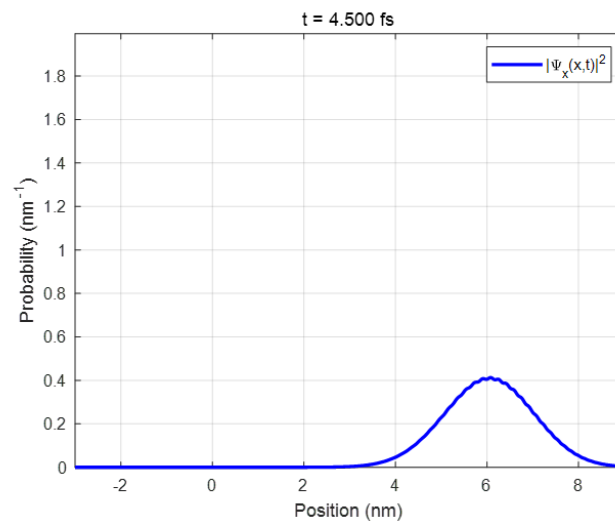
Plots the total and potential energy.



Running the script yields a total energy of 12 and a potential energy of 0

FLAG\_plot\_PS\_Position(line 27)

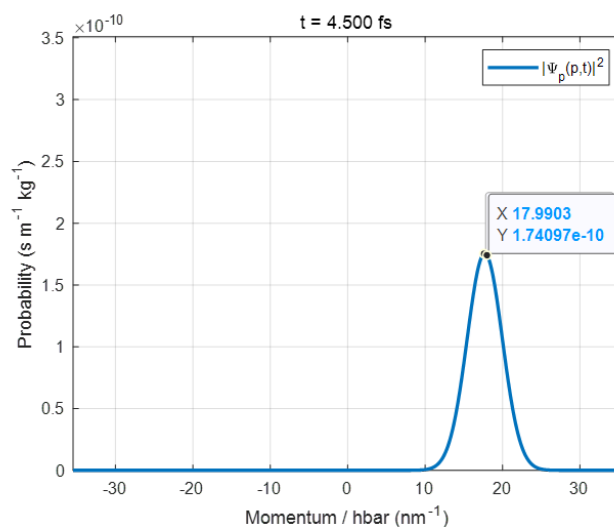
Plots the wavefunction for Position:  $\Psi_x(x, t)$



Run the script to get the wave function of the drawing position:  $\Psi_x(x, t)$  at 6nm max is 0.4

FLAG\_plot\_PS\_Momentum(line 31)

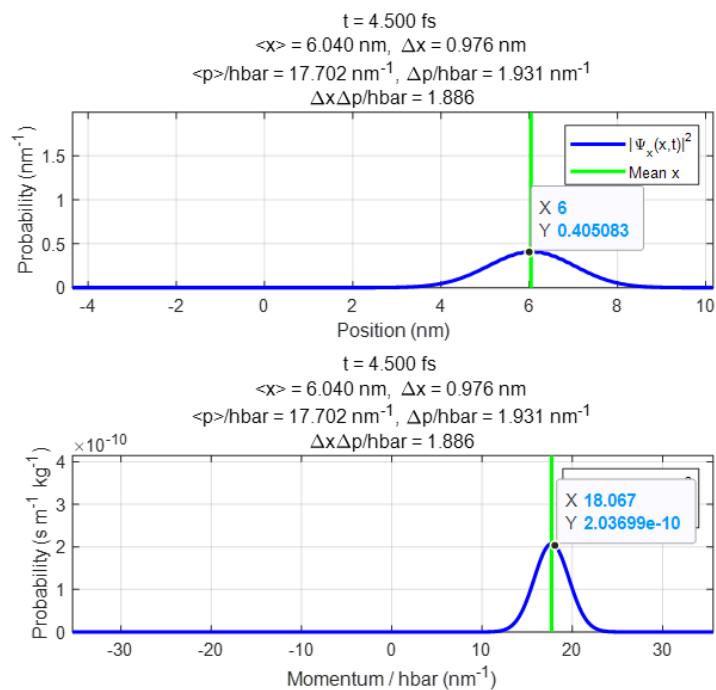
Plots the wavefunction for Momentum:  $\Psi_p(p, t)$



Run the script to draw the momentum of the wave function:  $\Psi_p(p, t)$  at 17.9903 nm has max value 1.74097 e-10

FLAG\_plot\_Mean\_Expectation\_Value(line 35)

Plots the mean values of position or momentum.

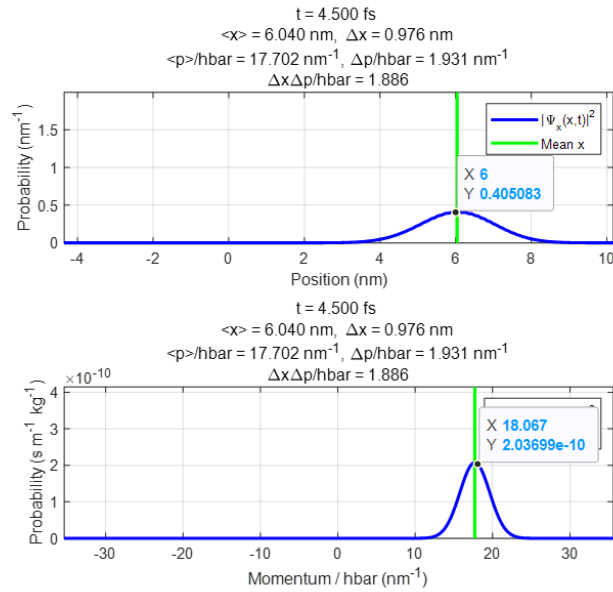


Running the script results in a drawing position at 6 nm

Average value of momentum 18.067 $\hbar$

FLAG\_calculate\_expectation\_values(line 37)

Calculates expectation values (displays mean  $x$  and  $\Delta x$ ).

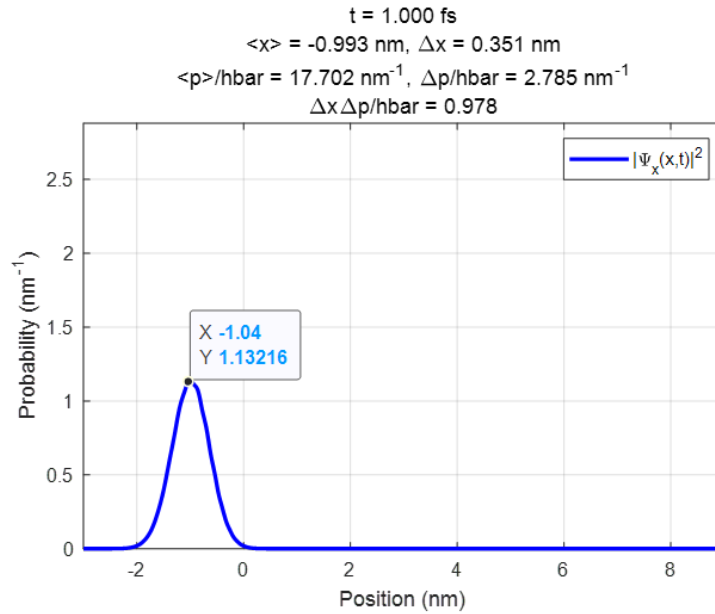


mean  $x = 6.04 \text{ nm}$ ,  $\Delta x = 0.976 \text{ nm}$

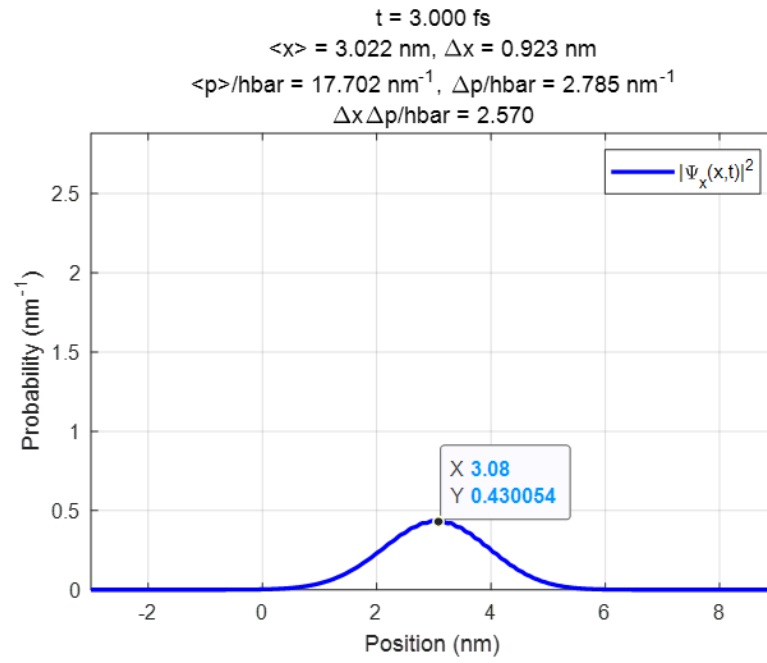
2(a)

an average / typical wavelength =  $3.5426\text{e-}10$

2(b)



At  $t = 1 \text{ fs}$ , spatial probability density is  $x = -0.993 \text{ nm}$ ,  $\Delta x = 0.351 \text{ nm}$ ,  $Y = 1.13216 \text{ nm}^{-1}$



At  $t = 3 \text{ fs}$ , spatial probability density is  $x = 3.022 \text{ nm}$ ,  $\Delta x = 0.923 \text{ nm}$ ,  $Y = 1.13216 \text{ nm}^{-1}$

**2(c)**

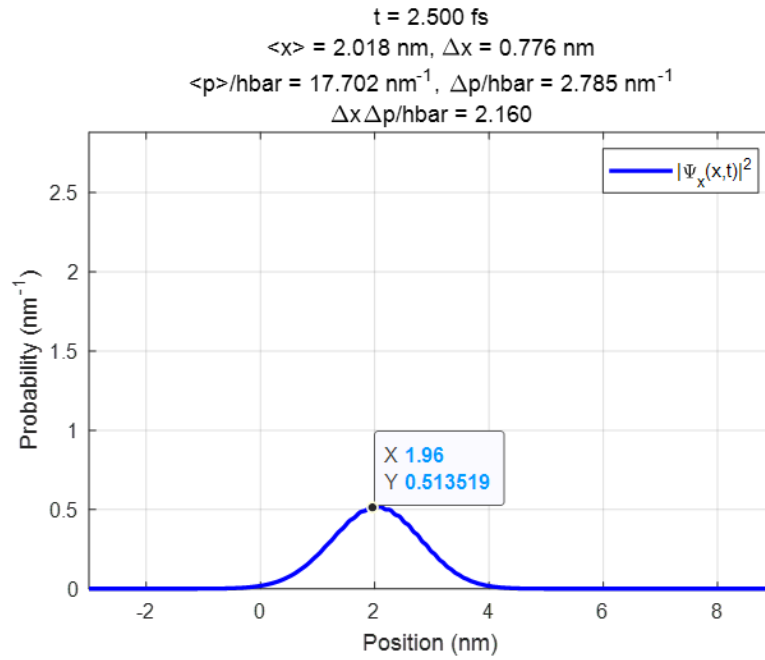
Group Velocity  $v = \hbar k / m = \hbar \pi / m \lambda_o = 6.626 \times 10^{-34} \times \pi / 9.11 \times 10^{-31} \times 3.5426 \times 10^7 = 2.28 \times 10^7 \text{ (nm/fs)}$

**2(d)**

Phase Velocity  $v = \hbar k / 2m = \sqrt{E / 2m} = 1.14 \times 10^7 \text{ (nm/fs)}$

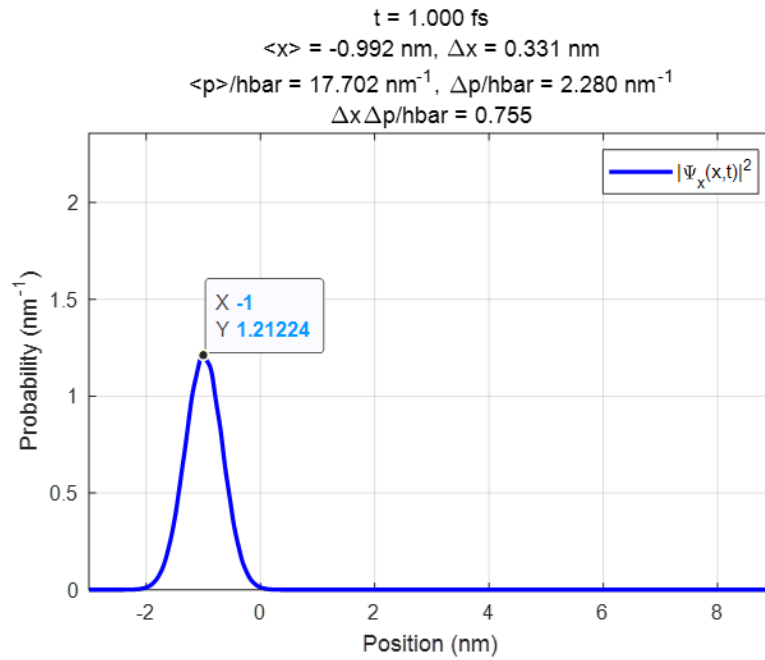


2(e)

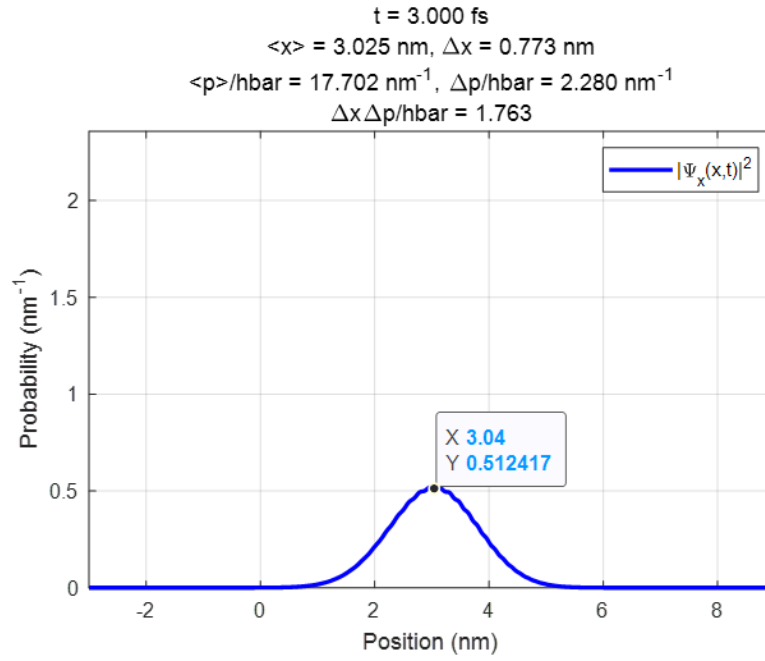


At  $t = 2.5 \text{ fs}$ , spatial probability density is  $x = 2.018 \text{ nm}$ ,  $\Delta x = 0.776 \text{ nm}$ ,

2(f)



At  $t = 1 \text{ fs}$ , spatial probability density is  $x = -0.992 \text{ nm}$ ,  $\Delta x = 0.331 \text{ nm}$ ,  $Y = 1.21224 \text{ nm}^{-1}$



At  $t = 3 \text{ fs}$ , spatial probability density is  $x = 3.025 \text{ nm}$ ,  $\Delta x = 0.773 \text{ nm}$ ,  $Y = 0.512417 \text{ nm}^{-1}$

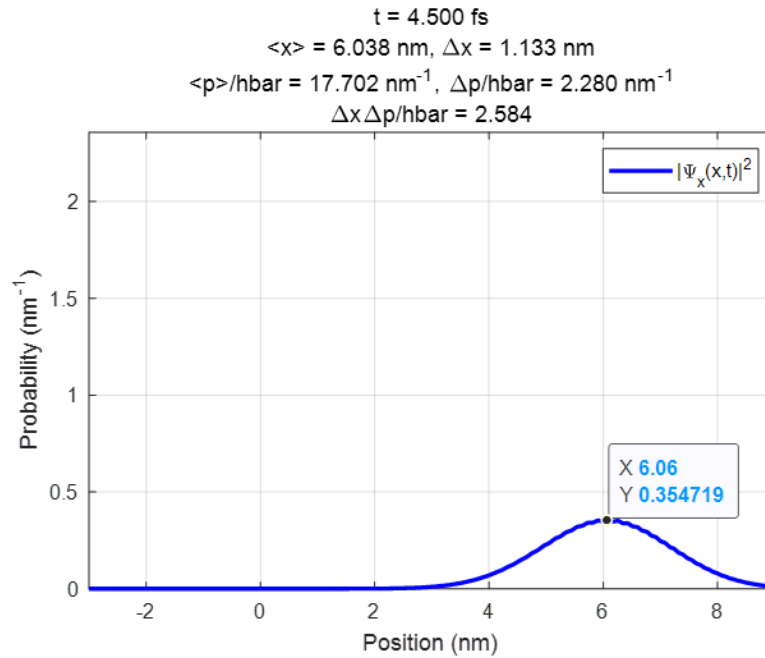
Compared with the findings in 2b), we know at  $\Delta x = 0.18$ , and at  $t = 1 \text{ fs}$ , spatial probability density is  $x = -0.993 \text{ nm}$ ,  $\Delta x = 0.351 \text{ nm}$ ,  $Y = 1.13216 \text{ nm}^{-1}$ , at  $t = 3 \text{ fs}$ , spatial probability density is  $x = 3.022 \text{ nm}$ ,  $\Delta x = 0.923 \text{ nm}$ ,  $Y = 1.13216 \text{ nm}^{-1}$ ,

Re-set the initial spatial uncertainty to  $\Delta x = 0.22$  (line 10).

At  $t = 1 \text{ fs}$ , spatial probability density is  $x = -0.992 \text{ nm}$ ,  $\Delta x = 0.331 \text{ nm}$ ,  $Y = 1.21224 \text{ nm}^{-1}$ , at  $t = 3 \text{ fs}$ , spatial probability density is  $x = 3.025 \text{ nm}$ ,  $\Delta x = 0.773 \text{ nm}$ ,  $Y = 0.512417 \text{ nm}^{-1}$

The comparison results show that  $\Delta x$  increase  $0.22 - 0.18 = 0.04$ , At  $t = 1 \text{ fs}$ , spatial probability density  $x$  decrease  $0.001 (0.992 - 0.993 = -0.001)$ ,  $\Delta x$  decrease  $0.02 (0.331 - 0.351 = -0.02)$ ; At  $t = 3 \text{ fs}$ , spatial probability density  $x$  increase  $0.003 (3.025 - 3.022 = 0.003)$ ,  $\Delta x$  decrease  $0.15 (0.773 - 0.923 = -0.15)$ .

2(g)



$t = 4.5 \text{ fs}$ , spatial probability density is  $x = 6.038$ ,  $\Delta x = 1.133 \text{ nm}$ ,  $Y = 0.3546 \text{ nm}^{-1}$

At  $t = 4.5 \text{ fs}$ , The resultant wavefunction shifts to the right and the amplitude becomes smaller.

|     |                                 | Experimental          | Theoretical         |
|-----|---------------------------------|-----------------------|---------------------|
| (a) | $\lambda$                       | $3.5426 \text{ e-}10$ | $3.54 \text{ e-}10$ |
| (b) | $\Delta x(t = 1 \text{ fs})$    | 0.331                 | 0.335               |
|     | $\Delta x(t = 3 \text{ fs})$    | 0.773                 | 0.776               |
| (c) | $vg[\text{nm/fs}]$              | $2.28 \cdot 10^7$     | $1.987 \cdot 10^7$  |
| (d) | $v\phi[\text{nm/fs}]$           | $1.14 \cdot 10^7$     | $0.9935 \cdot 10^7$ |
| (e) | $\Psi_x(x, t = 2.5 \text{ fs})$ | 0.603                 | 0.601               |

In the particle description of matter, matter particles have precisely defined locations and trajectories in space, but particle-related waves of matter seem to extend throughout space like ripples in a pond.

In quantum mechanics, we use local wave functions (also known as wave packets) to capture both the particle and the wave properties of particles.

Fourier transform transfers the wave packet from its position  $x$ - representation ( $x$ ) to its momentum  $p$ - representation ( $p$ ). Gaussian wavepackets are commonly referred to as Fourier limited wavepacket shapes, it is uncertain to represent real electrons, so the Fourier Series is better at representing real electrons (particles).