

Lab # 2

Wavepacket Collision and Bound States

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David Li

1006940134

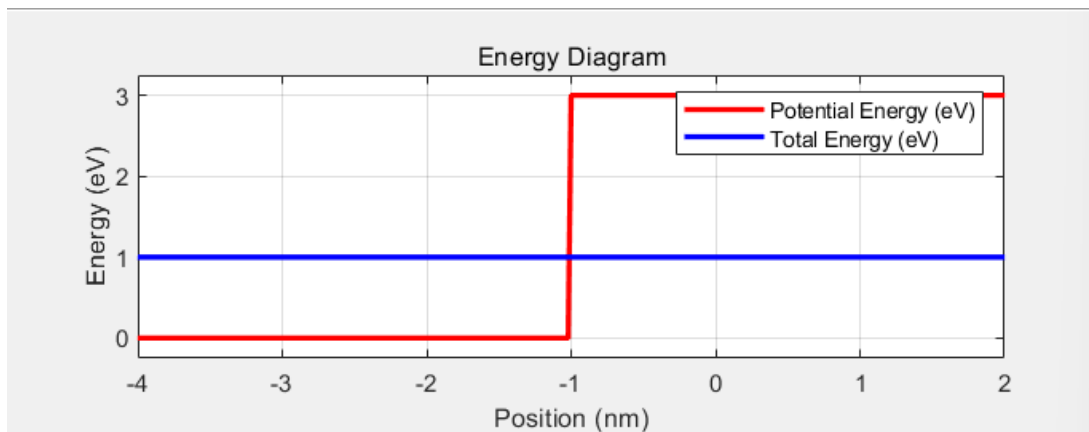
The Edward S. Rogers Sr. Department of Electrical & Computer Engineering
University of Toronto

1 Wave packet Collision with Potential Step

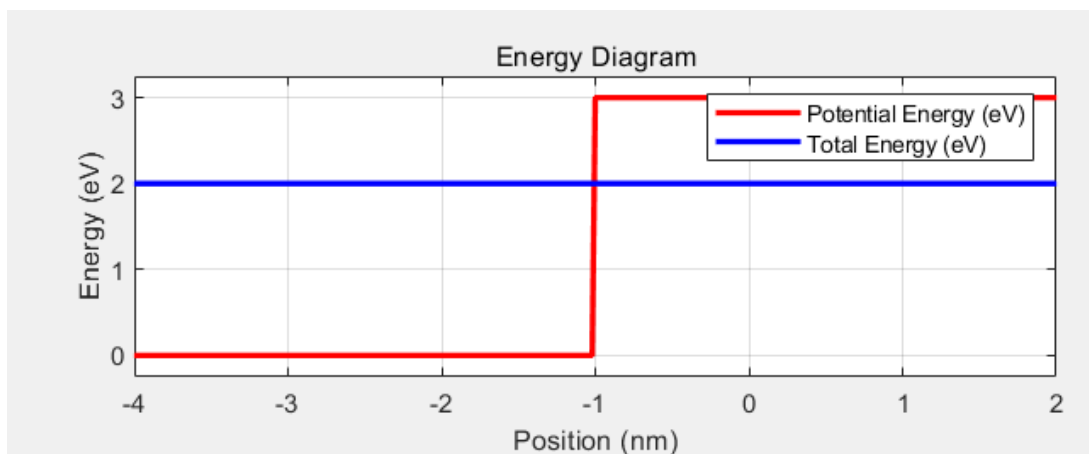
$$V = \begin{cases} 0 \text{ eV}, & x < -1 \text{ nm} \\ 3.0 \text{ eV}, & x \geq -1 \text{ nm} \end{cases}$$

(a)

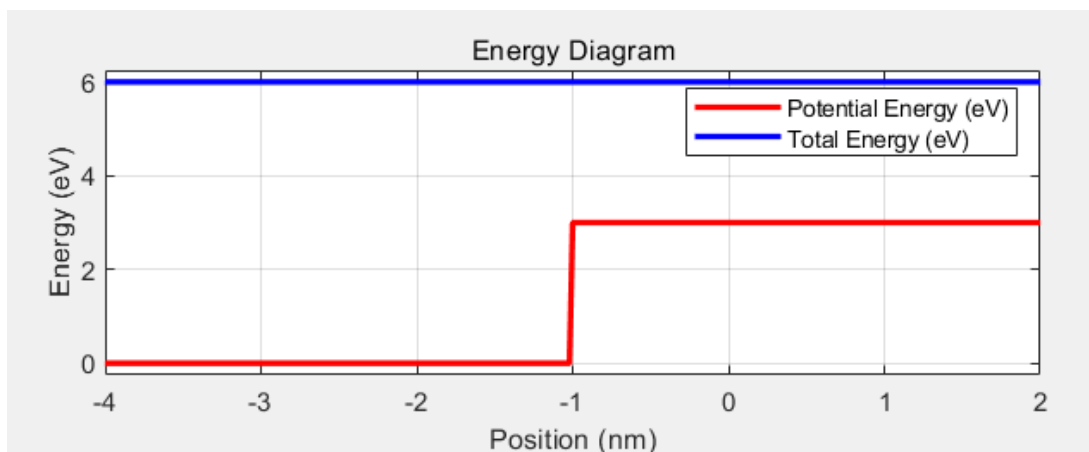
$$\langle E \rangle = 1 \text{ eV}$$



$$\langle E \rangle = 2 \text{ eV}$$



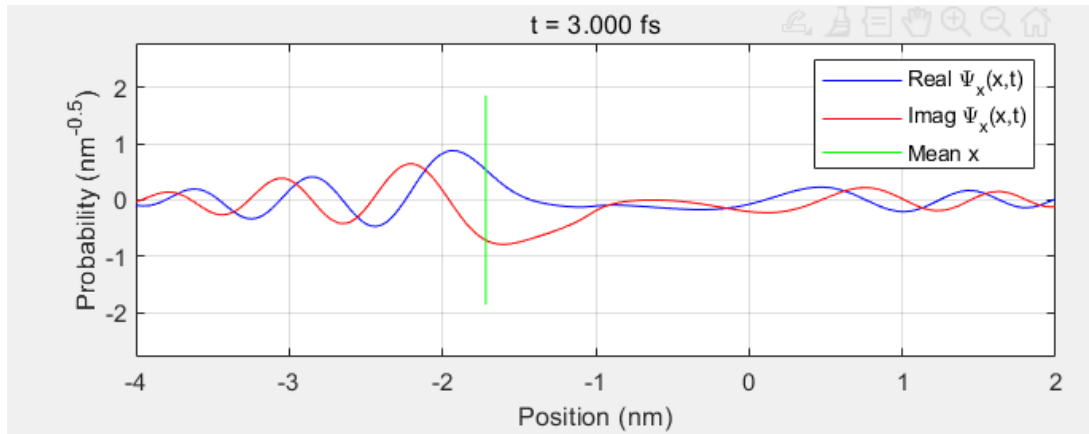
$$\langle E \rangle = 6 \text{ eV}$$



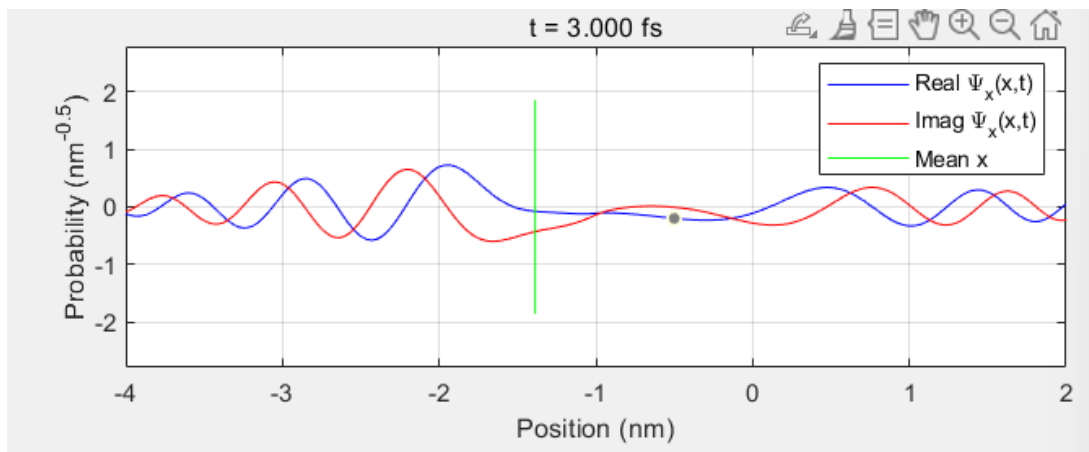
As the particle energy increases to 3 eV, it reaches the potential step, after which the particle energy increases beyond the potential step.

(b)

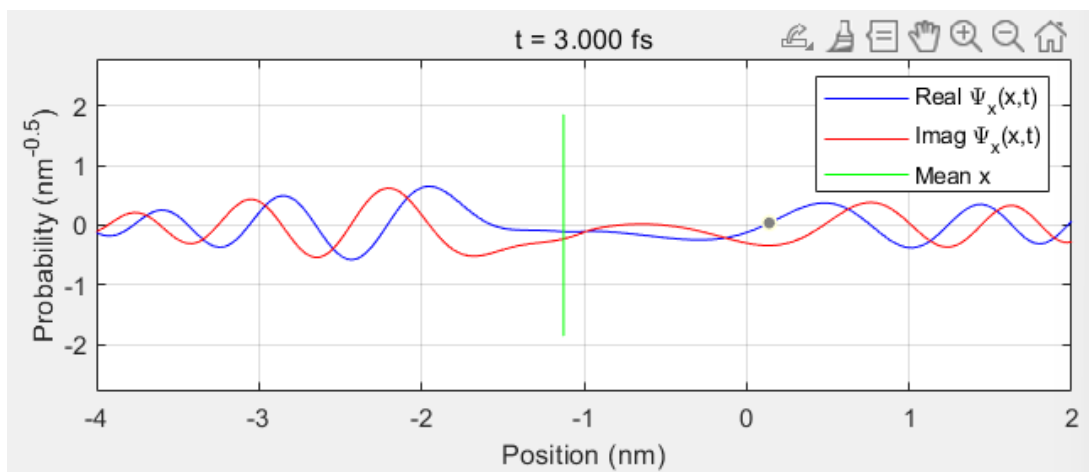
$$\langle E \rangle = 1.0 \text{ eV}$$



$$\langle E \rangle = 2.0 \text{ eV}$$

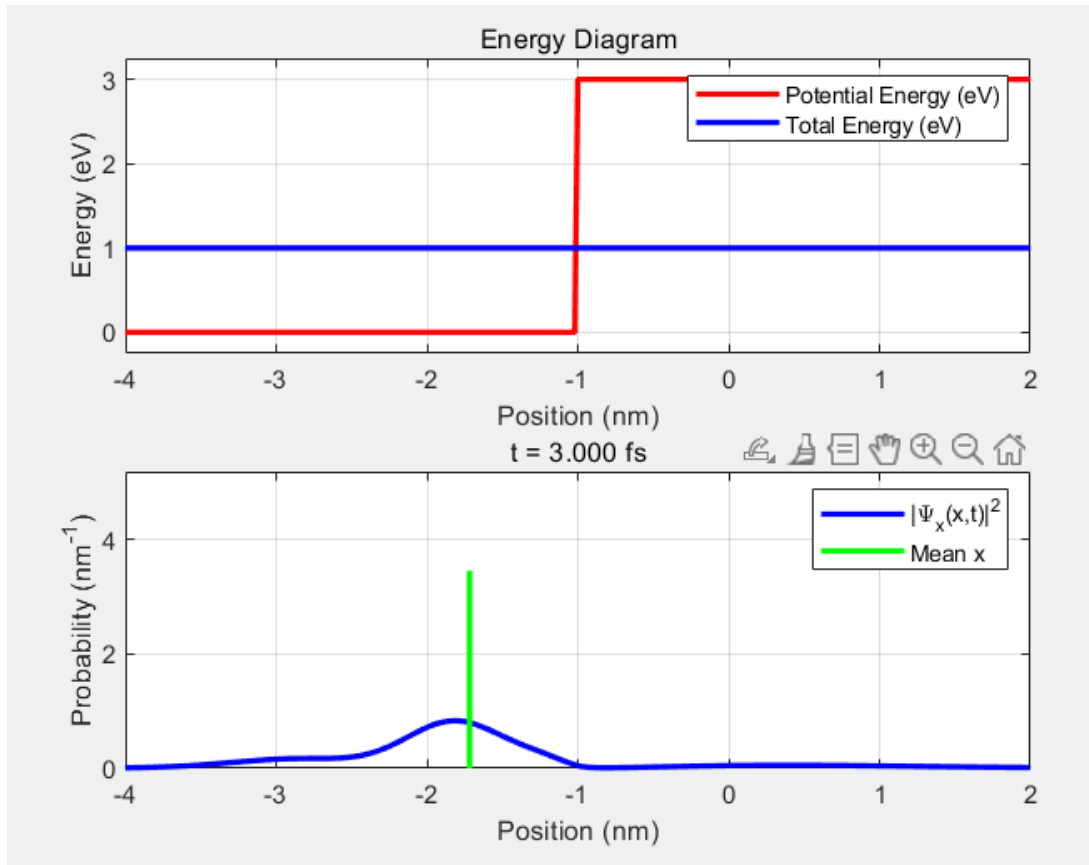


$$\langle E \rangle = 2.5 \text{ eV}$$



(c)

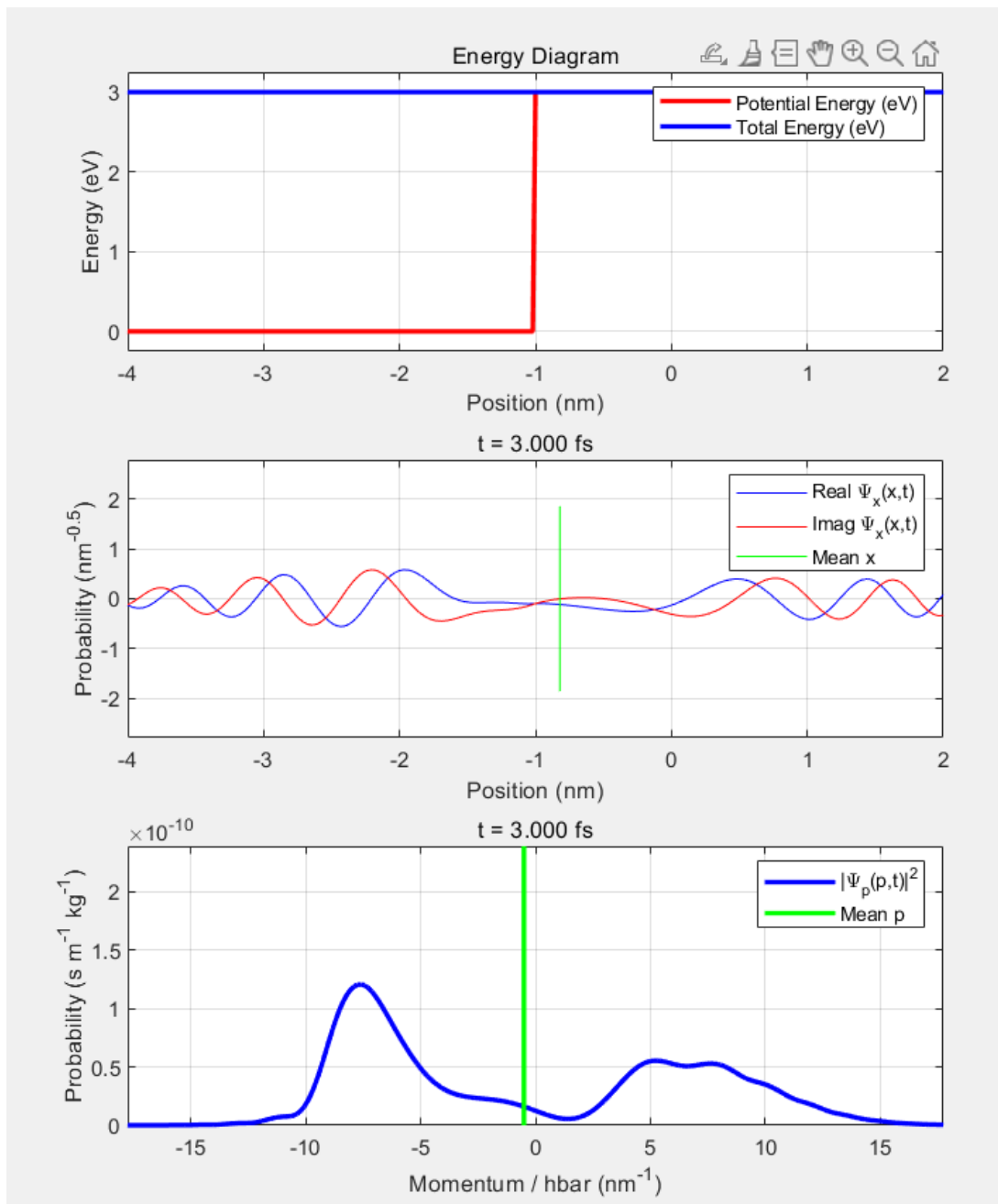
In classical physics, when potential energy is less than the step, it cannot penetrate through, or the region inside the barrier is classically forbidden, however, in quantum physics the wavefunction is continuous at the step and gets partially transmitted.



(d)

$\langle E \rangle = 1 \text{ eV}, x = -0.1 \text{ nm}$ The average energy of the incident wave packet is lower than 3.0 eV	
$\langle E \rangle = 2 \text{ eV}, x = -0.1 \text{ nm}$	
$\langle E \rangle = 3 \text{ eV}, x = -0.1 \text{ nm}$	
$\langle E \rangle = 4 \text{ eV}, x = -0.1 \text{ nm}$ The average energy of the incident wave packet is higher than 3.0 eV	
$\langle E \rangle = 5 \text{ eV}, x = -0.1 \text{ nm}$	
$\langle E \rangle = 6 \text{ eV}, x = -0.1 \text{ nm}$	

(e)



The waveform shows that this is a 50/50 transmission/reflection condition

(f)

Image of step potential position starting from -2 nm

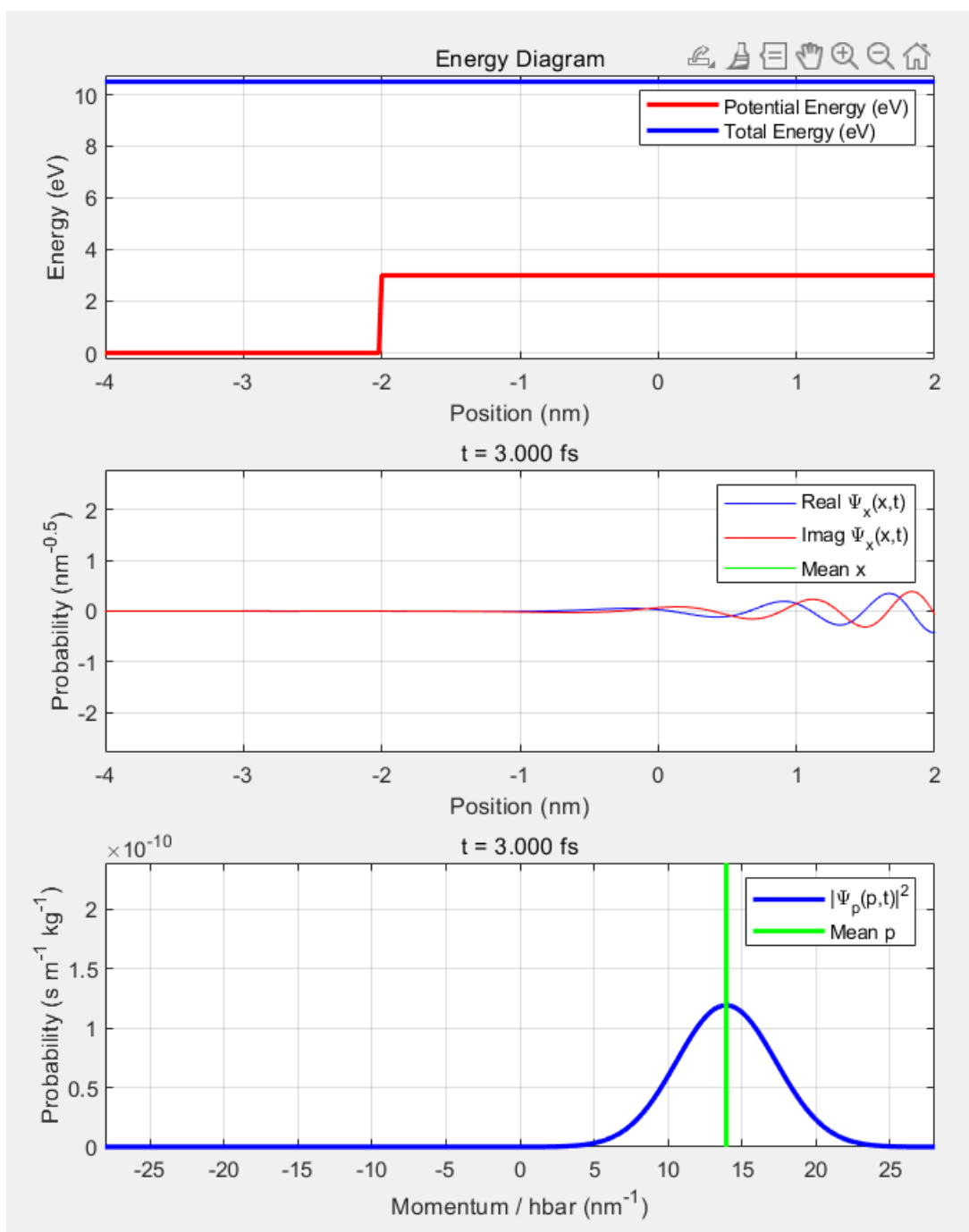


Image of step potential position starting from 0 nm

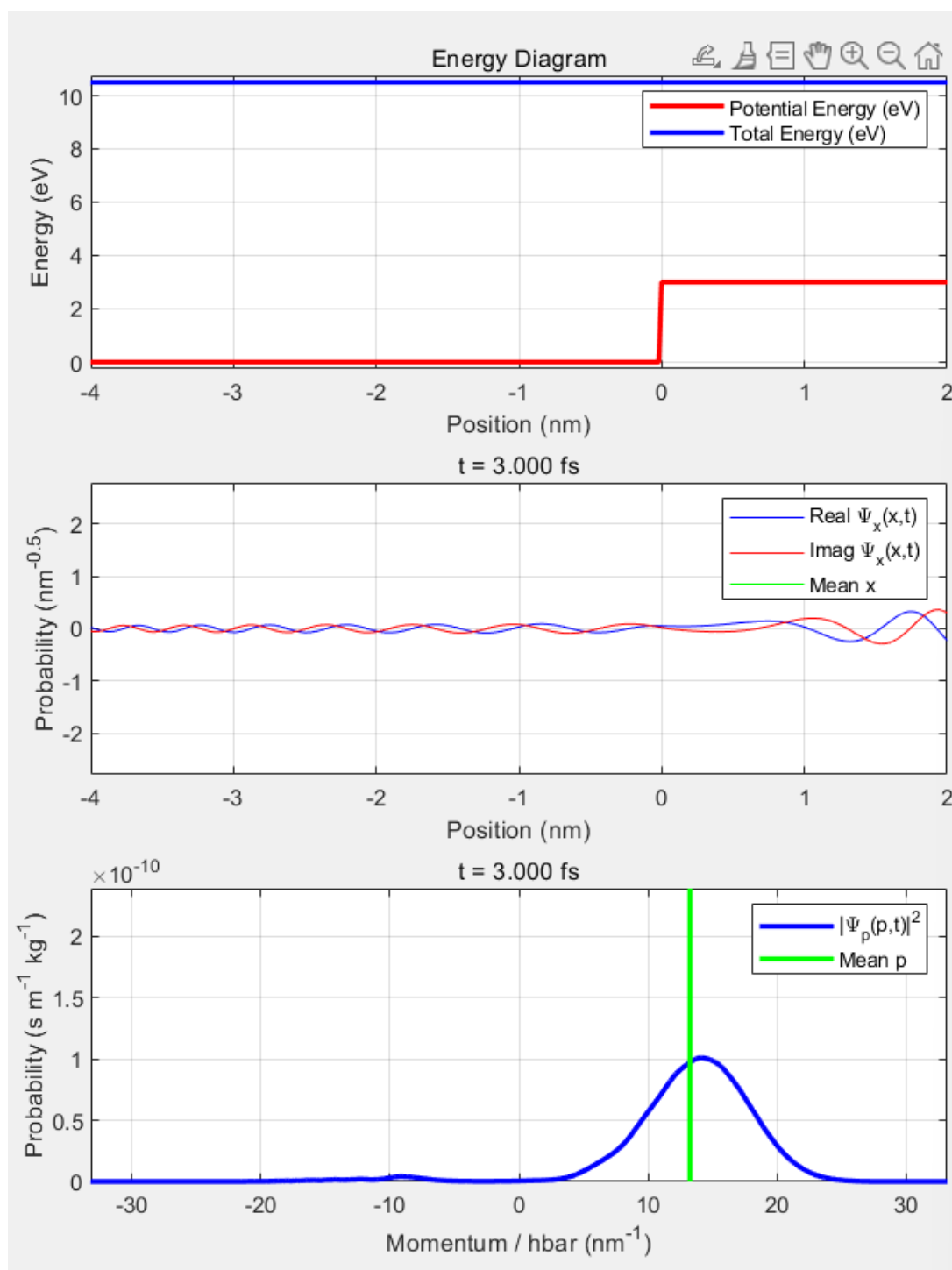
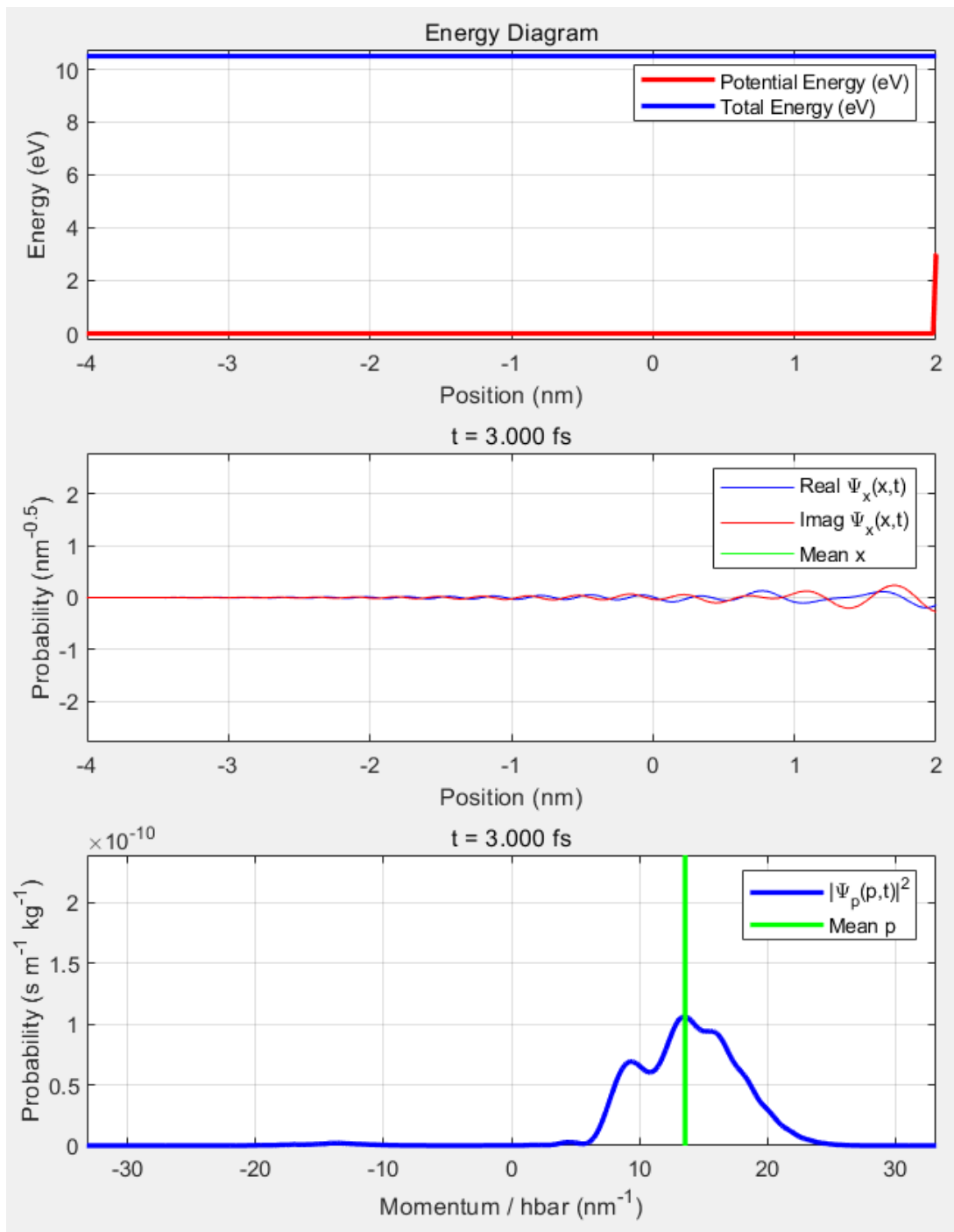


Image of step potential position starting from 2 nm

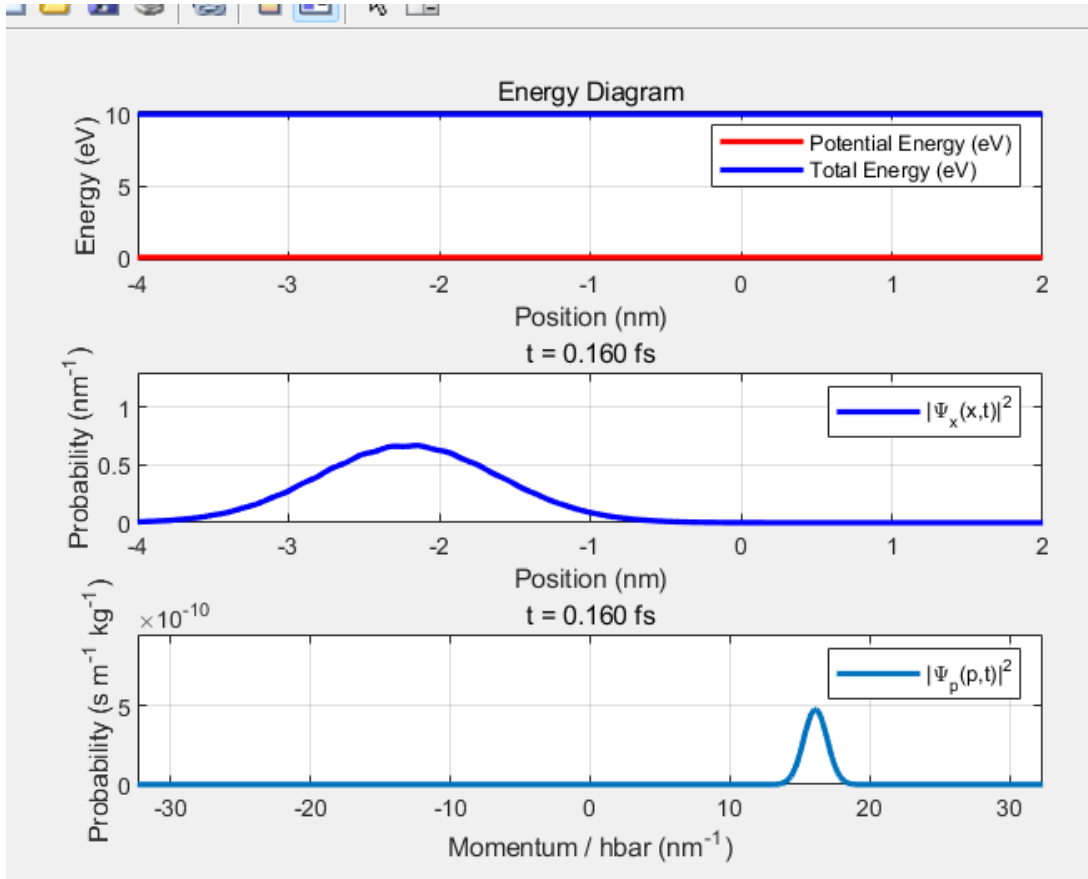


The particle velocity and average wavelength values also changes if changing the step potential position.

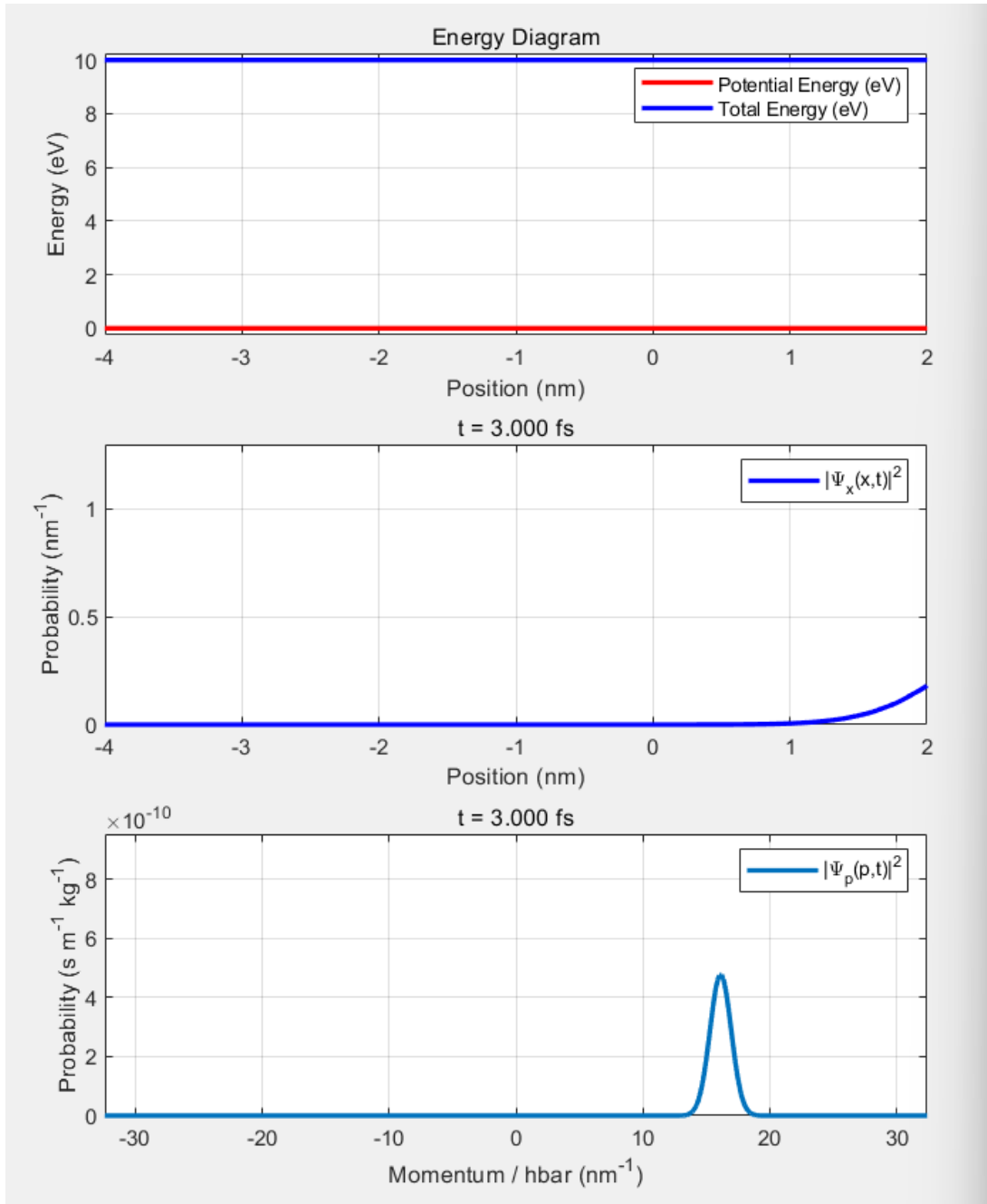
2 Wave packet Collision with Potential Barrier

$$V(x) = \begin{cases} 0\text{eV}, & x < 0 \text{ nm} \\ 17\text{eV}, & 0 \text{ nm} \leq x < 0.5 \text{ nm} \\ 0\text{eV}, & 0.5 \text{ nm} \leq x \quad (0.5 \text{ nm width}) \end{cases}$$

(a)



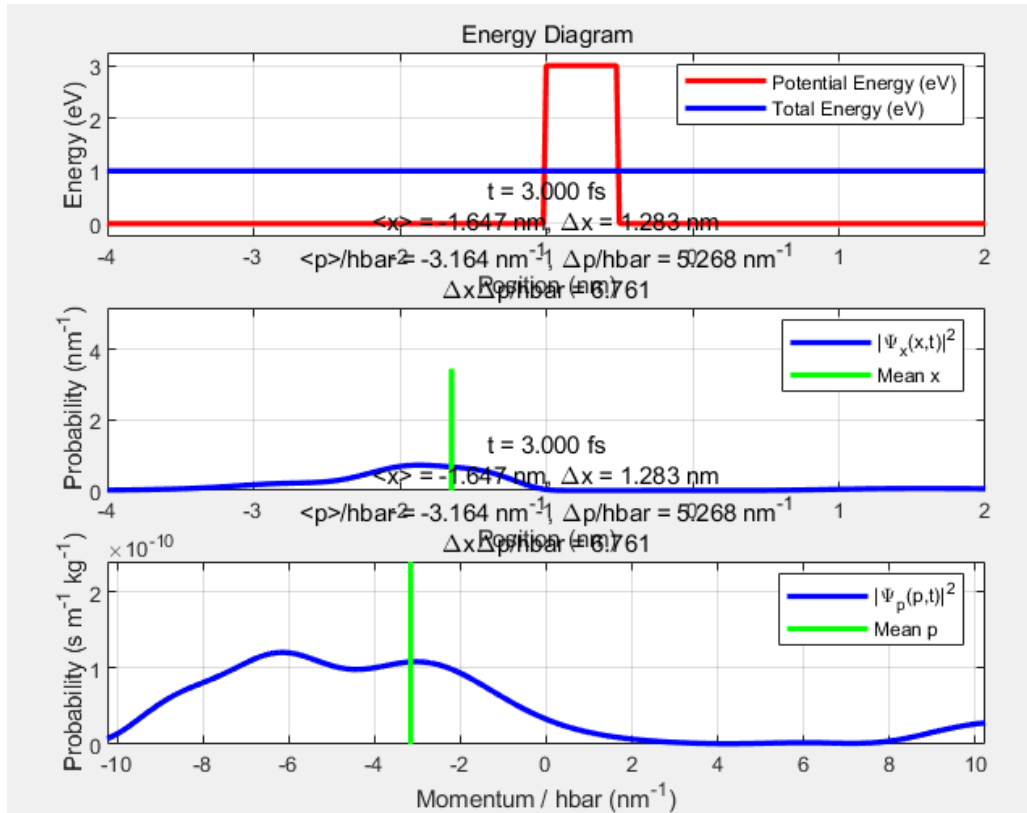
At $t = 0.16 \text{ fs}$, wavefunction is between -3 and -1



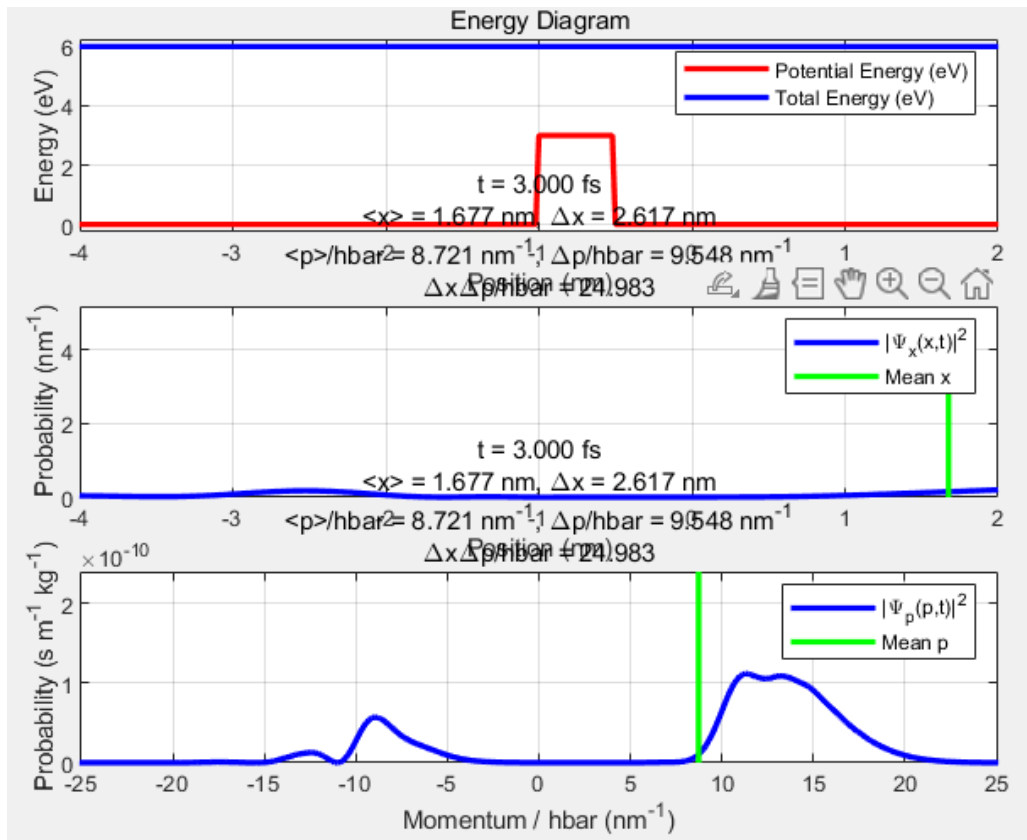
At $t = 3$ fs, The wave function wave moves to the right at a position greater than 1 as the simulation time increases

(b)

$$\langle E \rangle = 1 \text{ eV}$$

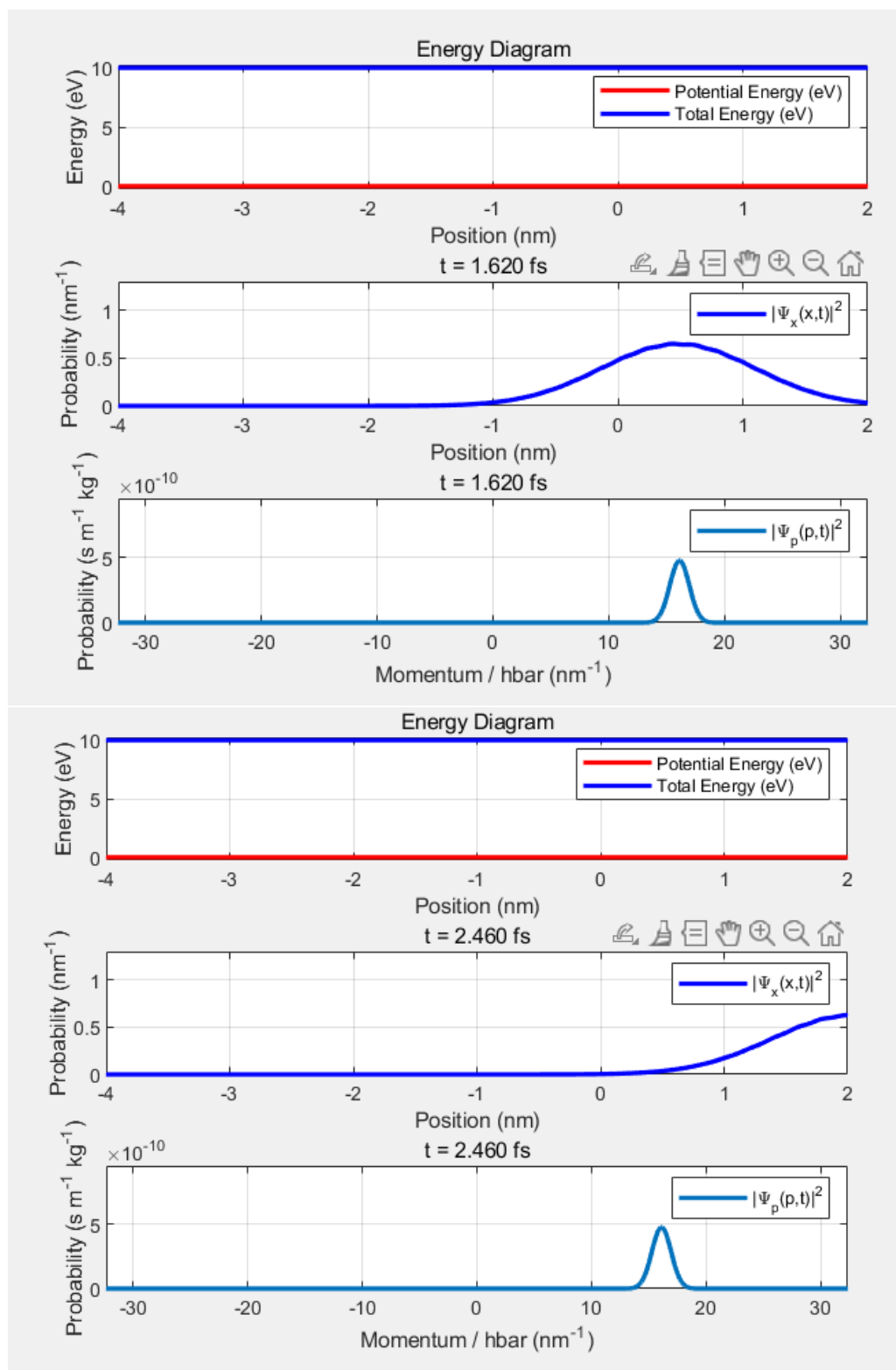


$$\langle E \rangle = 6 \text{ eV}$$

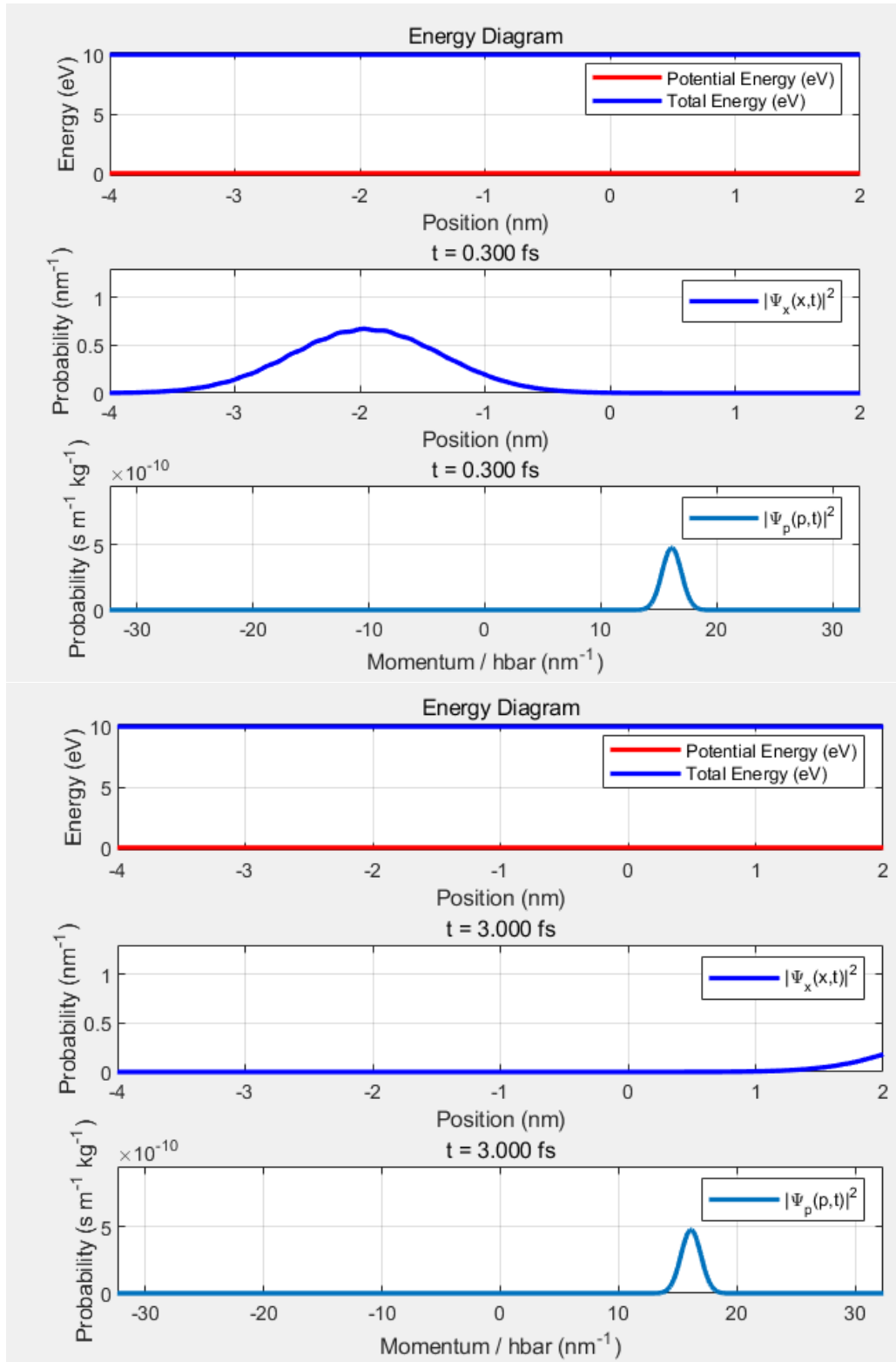


(c)

Wave packet evolution of barrier width 0.5 nm



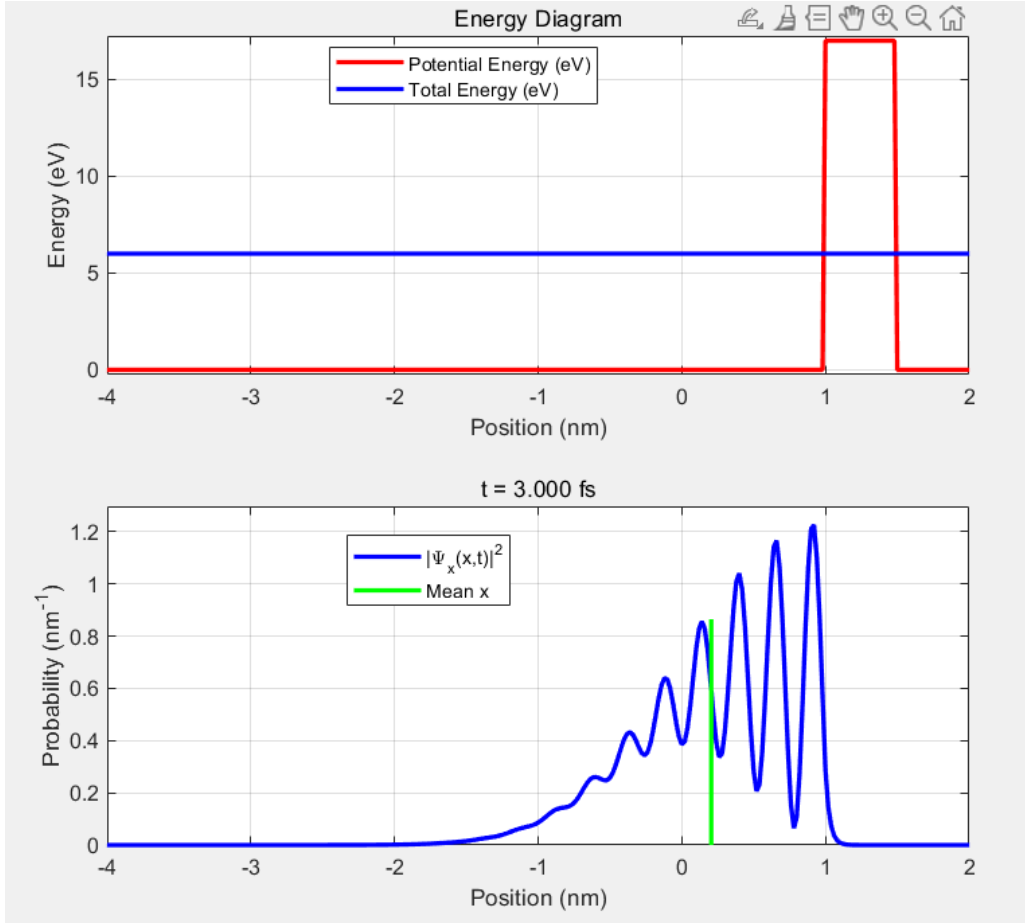
Wave packet evolution of barrier width 0.05 nm



3 Bound Energy States of a Symmetric Quantum Well

(a)

When $a = 1$ nm, $A = 1$, $B = 1$, $E_o = 6.0$, $m = 9.11 \times 10^{-31}$, $\hbar = 6.626 \times 10^{-34}$;



From simulation $\Psi(x)$ has max amplitude 1.2, and $1 > x > 0$, calculation $k = \sqrt{2 * m * (E + V_0)} / h = 6.4735 * 10^{-15} / 6.626 * 10^{-34} = 0.977 * 10^{19}$.

$$\Psi(x) = B \cos(kx) = \cos(k * 1 * 10^{-9}) = \cos(0.977 * 10^{19}) = 0.9988$$

(b)

Due to the limiting effect of potential Wells, the energy of electrons or holes in each potential well moving perpendicular to the junction plane is no longer continuous, and only a series of discrete band values can be taken.

(c) :

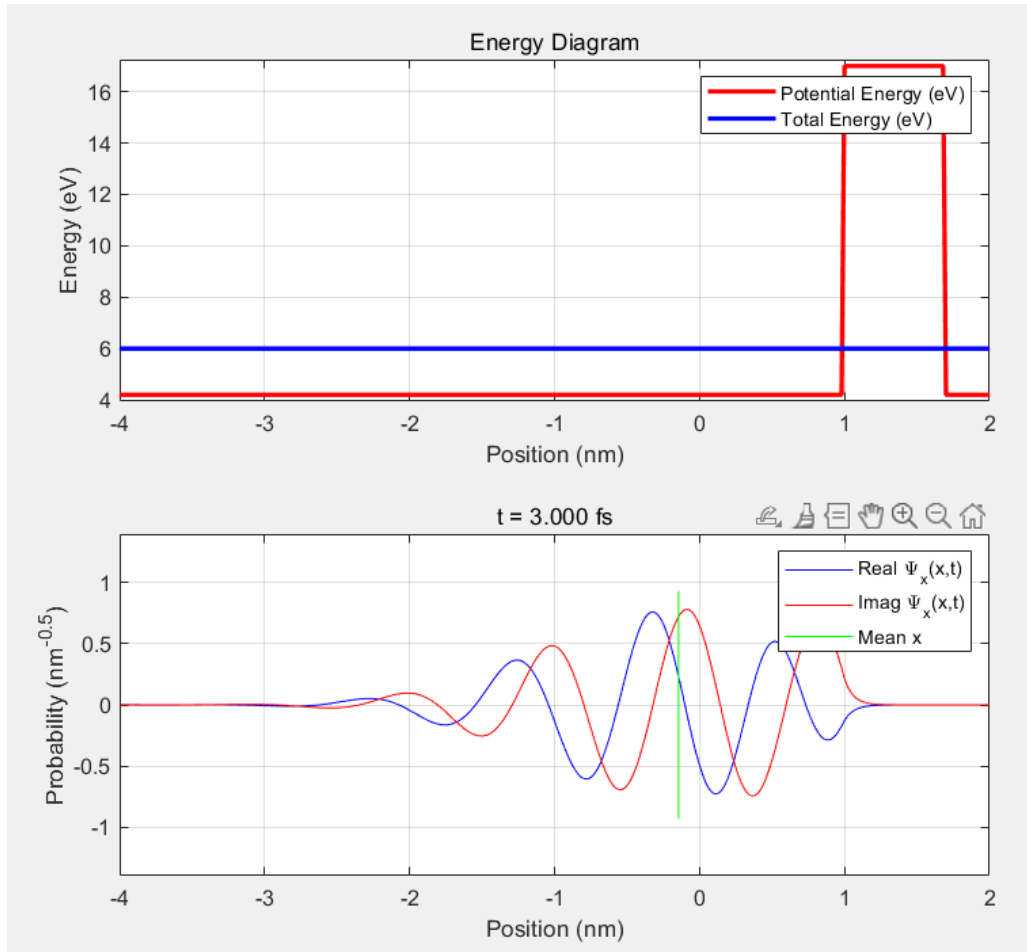
$$x = a = 1\text{nm},$$

$$z = k * a = (\sqrt{2 * m * (E + V_2)} / h) * 1 * 10^{-9} = 6.4735 * 10^{-15} * 1 * 10^{-9} = 6.4735 * 10^{-24}$$

$$z_0 = (a * \sqrt{2 * m * V_2}) / h = (1 * 10^{-9} * 5.5654 * 10^{-15}) / 6.626 * 10^{-34} = 0.839 * 10^{10}$$

$$\tan(z) = \sqrt{(z_0/z)^2 - 1} = 1.2961 * 10^{33}$$

(d)



From simulation $\Psi(x)$ has max amplitude 0.76, and $1 > x > 0$, calculate $k = \sqrt{2 * m * (E_o + V1)} / h = 3.3064 * 10^{-15} / 6.626 * 10^{-34} = 0.499 * 10^{19}$

$$\Psi(x) = B \cos(kx) = \cos(k * 1 * 10^{-9}) = \cos(0.499 * 10^{10}) = 0.9839$$

(e)

