DOING PHYSICS WITH PYTHON

QUANTUM MECHANICS

PARTICLE IN A BOX
[1D] FINITE SQUARE POTENTIAL WELL WITH A SLOPING FLOOR

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qm044.py **finite square well with sloping floor: RAMP POTENTIAL**

Solution of the [1D] Schrodinger equation by finding the eigenvalues and eigenvectors for an electron confined to a region of space by a finite square potential well with a sloping (ramp) floor.

GitHub

Google Drive

References

Operators, expectation values, Heisenberg Uncertainty Principle

Transverse standing waves

First and Second derivative operators

Bound particle: Eigenstates of a particle confined by a potential well

(eigenvalues and eigenvectors)

Bound particle: Square potential wells: finite and infinite

Bound particle: Square potential well with a sloping floor

Interesting Article

PHYSICAL REVIEW PHYSICS EDUCATION RESEARCH 15, 010139 (2019)

Graduate student misunderstandings of wave functions in an asymmetric well
C. D. Porter and A. F. Heckler

[1D] FINITE SQUARE WELL POTENTIAL WITH A SLOPING FLOOR

In this article we will consider a finite potential well with a sloping floor or ramp potential and the well is defined by the Python Code

qm044.py

```
xMin = -0.2*sx        #  default = -0.2 nm
xMax =  0.2*sx        #  default = +0.2 nm
U1 = -1200*se         #  Depth of well: default = -1200 eV
U2 = -200*se
w = 0.2*sx            #  Width of well: default 0.2 nm
# Potential energy function  [J]
U = zeros(N)
x1 = -(w/2); x2 = (w/2)
m = (U2-U1)/(x2-x1); b = U1 - m*x1
U[x>-w/2] = m*x[x>-w/2]  + b
U[x>w/2] = 0
UM = diag(U)
```

The well parameters were selected to give at least six eigenstates as shown in figure 1.

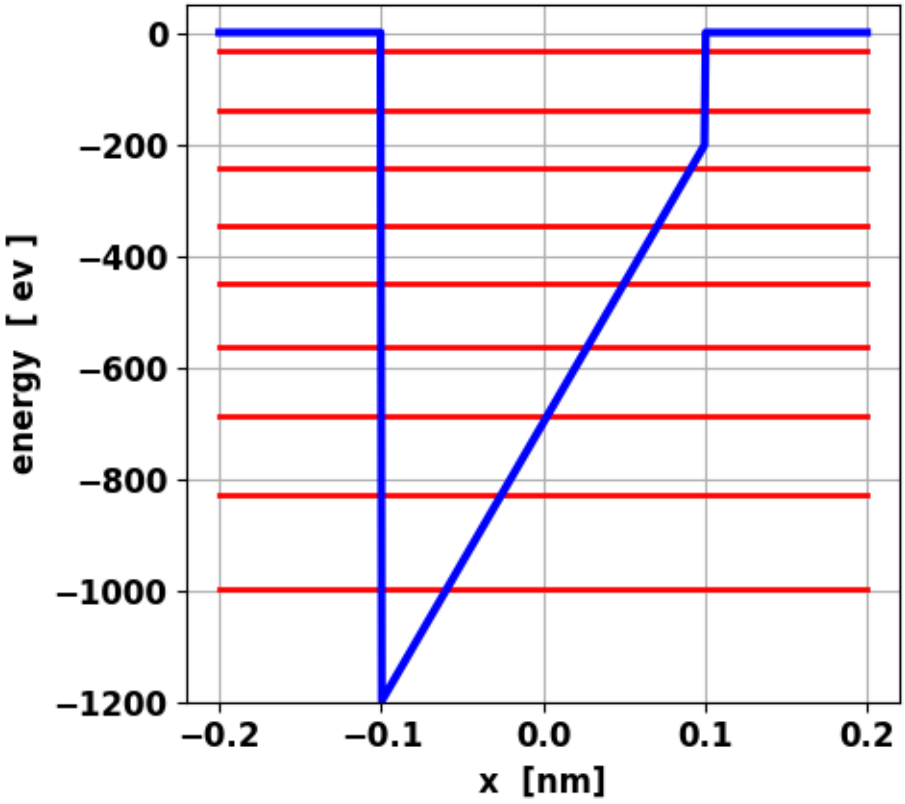

Fig. 1. Energy spectrum and square potential well with a sloping floor. The well parameters are: width w = 0.200 nm with depths U_1 = -1200 eV and U_2 = -200 eV.

Energy spectrum: energy eigenvalues [eV]

E1 = -998.987
E2 = -827.688
E3 = -687.575
E4 = -563.876
E5 = -450.941
E6 = -345.674
E7 = -244.537
E8 = -141.150
E9 = -33.763

Eigenfunctions (eigenvectors)

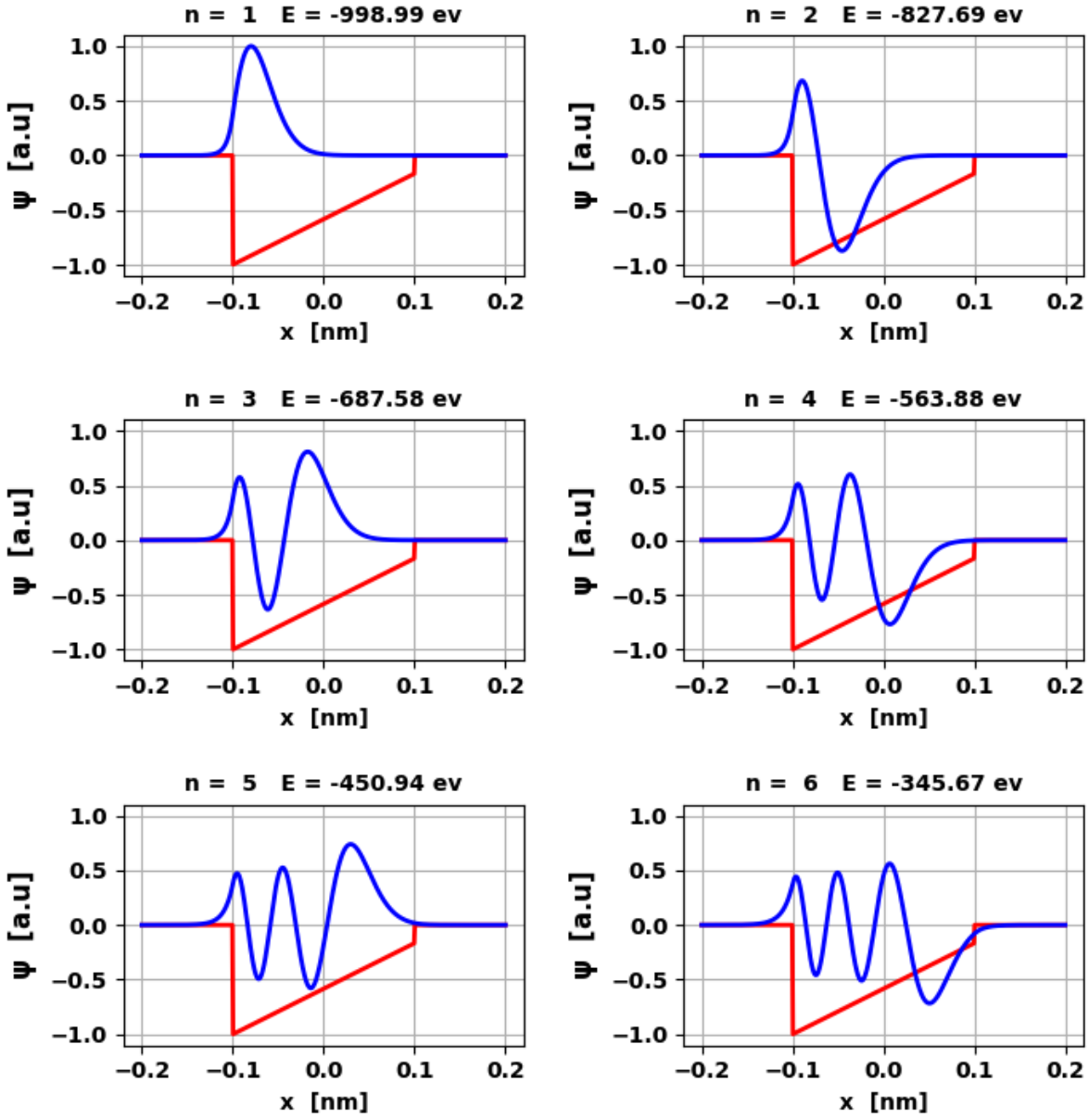

Fig. 2. Eigenfunctions for the **finite square well with a sloping floor** at time $t = 0$. Each eigenfunction has been scaled by dividing each eigenfunction by the maximum of eigenfunction $n = 1$. Note: The peaks in the eigenfunctions increase in height as the potential energy increases in the direction of increasing x.

Probability density functions

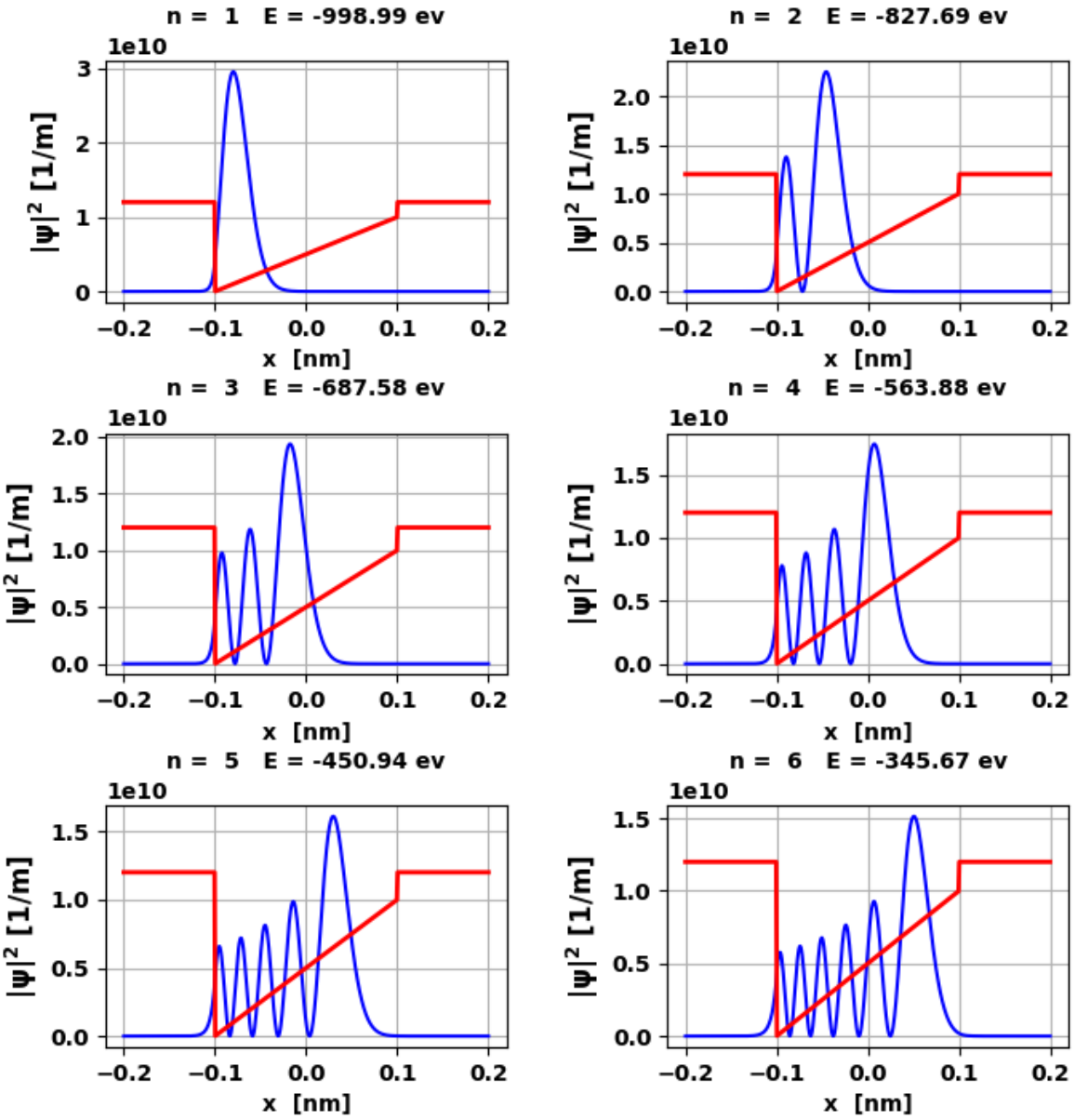

Fig. 3. Probability density function for the **finite square well with a sloping floor**. Area under curves is one since each eigenfunction has been normalized.

Quantum Interpretation

As the quantum number *n* increases, the maximum value in the amplitude of the eigenfunction shifts in the direction of higher potential energy and therefore, lower kinetic energy, lower momentum and longer wavelength.

This can be shown by considering the eigenfunction and its slope at the boundary between two adjacent sections. We can consider the eigenfunction to be expressed as a sine function, then

$$\psi = A\sin\left(\frac{2\pi}{\lambda}x+\phi\right) \quad \frac{d\psi}{dx} = \left(\frac{2\pi}{\lambda}\right)A\cos\left(\frac{2\pi}{\lambda}x+\phi\right) = m$$

$$A\sin\left(\frac{2\pi}{\lambda}x+\phi\right) = \psi \quad A\cos\left(\frac{2\pi}{\lambda}x+\phi\right) = \frac{m}{2\pi}\lambda \quad m \neq 0$$

These equations can be squared and added to eliminate the phase ϕ to give the equation for the maximum value of *A*

$$A = \sqrt{\psi^2 + \frac{m^2}{4\pi^2}\lambda^2}$$

At the boundary of the two adjacent sections, the eigenfunction ψ and its slope $m = d\psi / dx$ must be continuous function of *x*. So, at infinitesimal distances close to the boundary, the values of both ψ^2 and m^2 are equal in magnitude on either side, but the value of the wavelength increases in the direction of higher potential. Therefore,

the coefficient *A* increases with increasing wavelength, as shown in figure 2 for $n = 6$.

This result of greater amplitude with larger wavelength is important because any potential energy function can be approximated by a series of step functions. This implies that for any potential energy function, regions of smaller kinetic energy or smaller momentum and larger wavelength have a larger maximum value of the amplitude of the eigenfunction than adjacent regions of larger kinetic energy or momentum and smaller wavelength.

In nonuniform potential wells the wavefunctions are not sinusoidal, but over a small part of the cycle, the potential energy does not change much, and so we speak loosely of a local "wavelength".

Eigenstate explorations

In the input section of the code for **qm044.py** you can enter the quantum number *n* for the state. In running the Code, a summary of the expectation values is shown in the Console Window as well you can test the Uncertainty Principle

$$\Delta x \, \Delta p \geq \hbar / 2 \quad HUP = 2 \Delta x \, \Delta p / \hbar > 1.$$

Plots of the potential well, the eigenfunction and probability density are displayed in Figure Windows.

Eigenstate n = 2

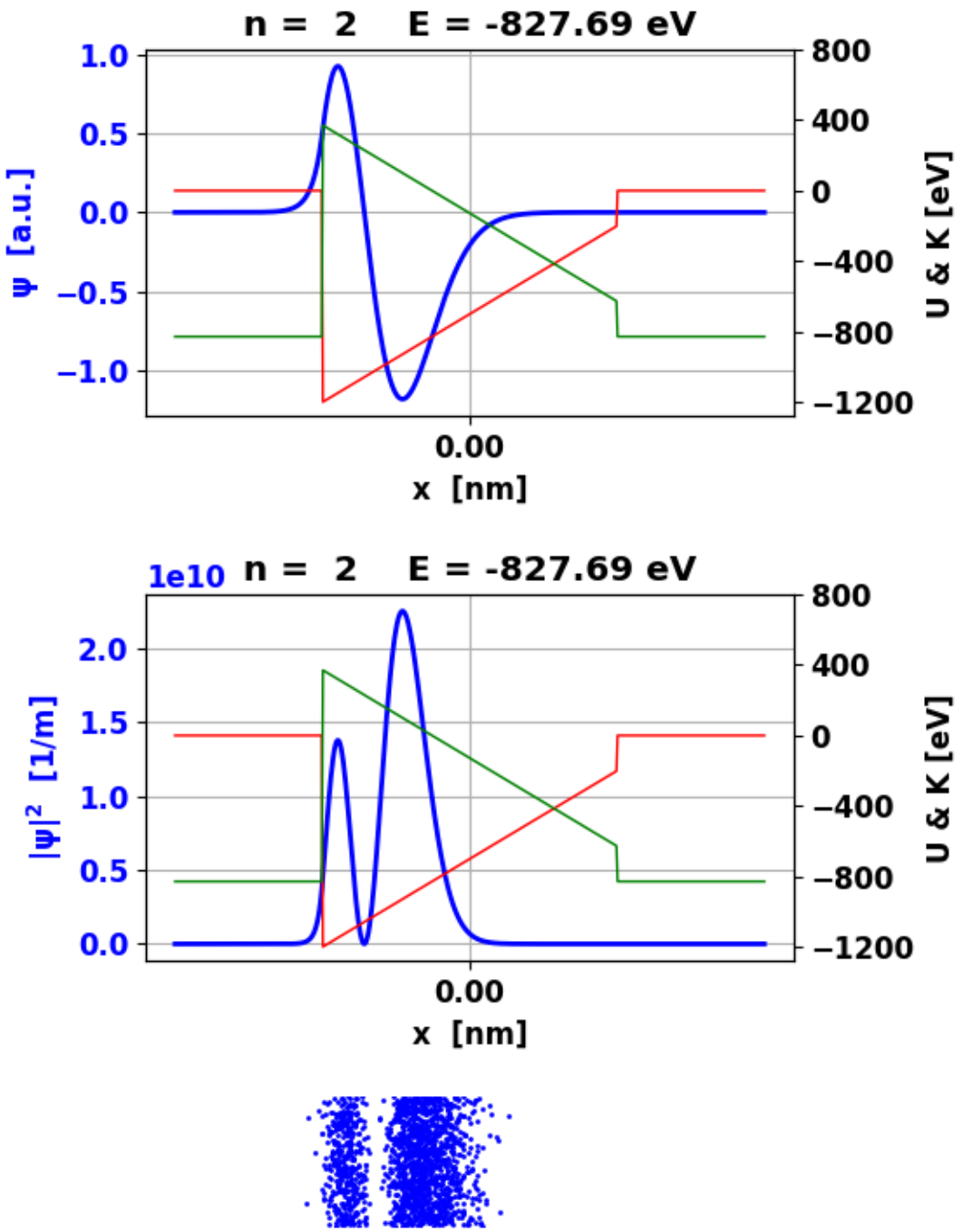

Fig. 4. $n = 2$: Plots of the eigenfunction, probability density and the potential energy function U and the kinetic energy function K. In the region where $K > 0$, the eigenfunction is a sinusoidal function (highest probability of finding the electron) and in the regions where $K < 0$, the eigenfunction is an exponentially decreasing function (non-zero probability of finding the electron).

Eigenstate n = 2

Expectation values and Uncertainty Principle

<x> = -0.053 nm

deltax dX = 0.024 nm

<p> = 0.00 N.s deltax dP = 5.87e-24 m

HUP = 2.70 > 1

Eigenstate energies

En = -827.69 eV

<E> = -827.69 <K> = 117.97 <U> = -945.66

<K> + <U> = -827.69

Execution time = 6 s

Eigenstate n = 6

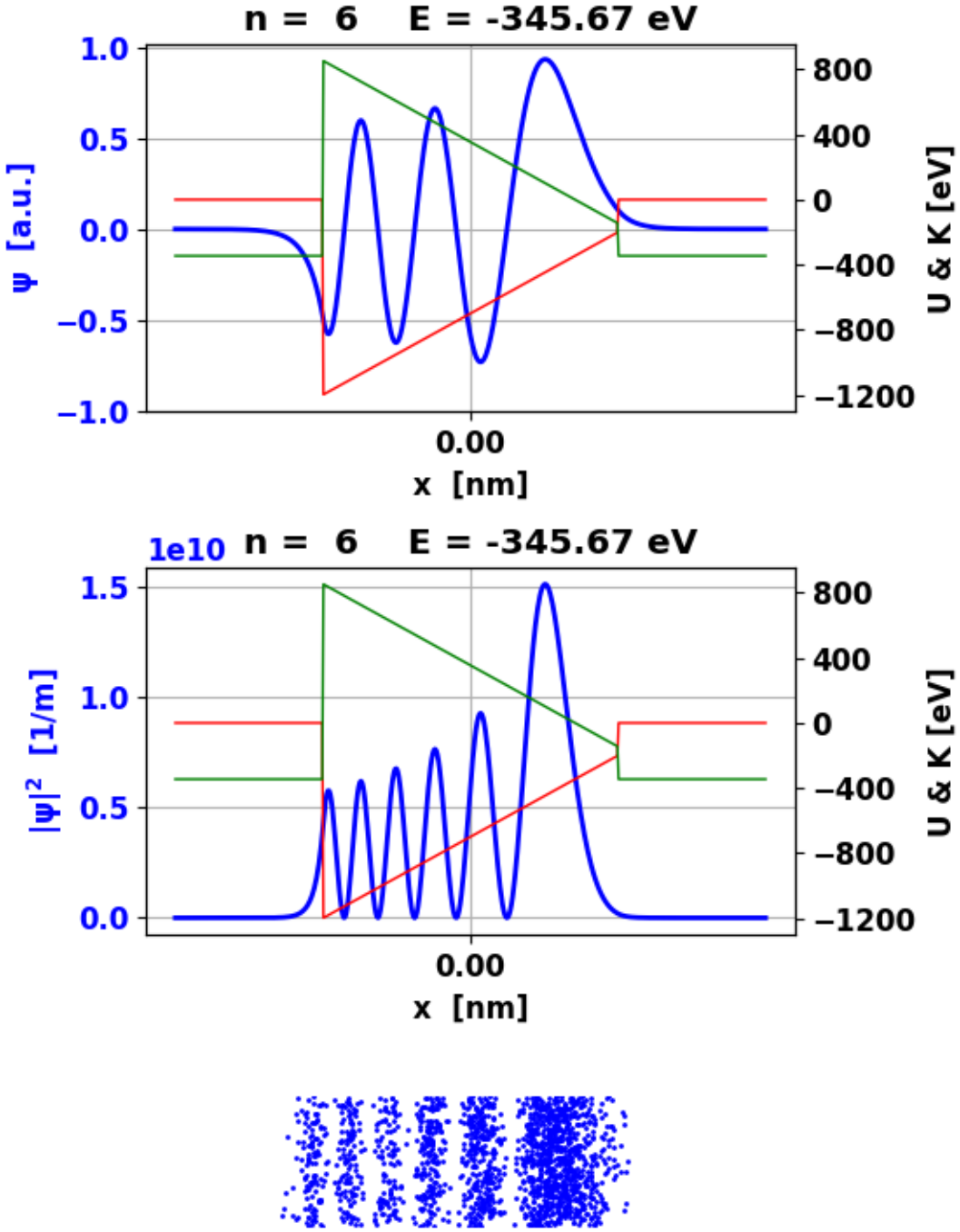

Fig. 5. n = 6: Plots of the eigenfunction, probability density and the potential energy function U and the kinetic energy function K. In the region where $K > 0$, the eigenfunction is a sinusoidal function (highest probability of finding the electron) and in the regions where $K < 0$, the eigenfunction is an exponentially decreasing function (non-zero probability of finding the electron).

Eigenstate n = 6
Expectation values and Uncertainty Principle
<x> = 0.010 nm
deltax dX = 0.054 nm
<p> = 0.00 N.s deltax dP = 9.01e-24 m
HUP = 9.21 > 1

Eigenstate energies
En = -345.67 eV
<E> = -345.67 <K> = 277.84 <U> = -623.52
<K> + <U> = -345.67

Execution time = 5 s