Wave Packets and Uncertainty Principle Worked Example

1. Suggested study steps, based on Feynman study model [a]

1. Read the statement of the problem
2. Read slowly through the solution to get the big picture.
3. With pencil, paper and calculator work through the self-explanation prompts.
4. Write a summary of the problem and the solution as you would explain it to a friend.

2. Statement of the problem

In quantum physics, a wave packet represents a quantum particle with quasi-spatial localization. Quai-spatial localization means the quantum particle can be described by the sum of harmonic functions, i.e. sinusoidal functions as $\psi(x) = \sin(kx) = \sin(px/\hbar)$. Any periodic wave $g(x)$ can be represented as a summation of harmonic related sinusoidal function, i.e. $g(x) = \sum_\alpha \sin(\alpha k_0 x) = \sum_\alpha \sin(\alpha p_0 x/\hbar)$. A mathematical framework to describe waves, periodic or nonperiodic, is the Fourier analysis and includes the Fourier series (periodic waves) and Fourier transformations (nonperiodic waves). The pair of variables defined in such way that they become Fourier transforms duals[b] are called conjugate variables[c], e.g. space (x)- momentum (p) and time (t) - energy (E). The uncertainty principle is applied only to conjugate variables and is an implication of the relation between these variables.

Suppose an electron in a quantum well of 4 nm of GaAs rounded by $Al_{0.3}Ga_{0.7}As$ as shown the figure 1. Suppose the wave function of the electron (without spin) can be approximated by,

$$\psi(x) = \begin{cases} \dfrac{\sqrt{2}}{2} \cos\left(n\dfrac{\pi}{4}x\right) & \forall\ |x| \le 2\ [nm] \\ 0 & \forall\ |x| > 2\ [nm] \end{cases}$$

where $n \in [1, \infty)$ and $n \in \mathbb{Z}$ is the quantum number that define the state of the system. What is the uncertainty to determine the position and momentum of the electron in the quantum well?

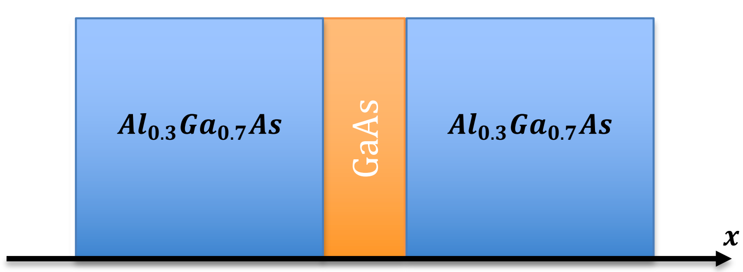


Figure 1. A quantum well of $Al_{0.3}Ga_{0.7}As$ / $GaAs$. For details see Paul Harrison, quantum wells, wires and dots, Willey (2005).

3. Strategy

In this problem, it is requested to calculate the uncertainty of position, x and momentum, $p = -i\hbar\frac{\partial}{\partial x}$, operators. To resolve this problem, it is necessary to define the uncertainty and calculate it.

4. Implementation

4.1. Uncertainty definition and methodology to calculate it

In physics uncertainty σ mean the precision to do a measure of a variable and is quantified by the standard deviation as,

$$\sigma_\alpha = \sqrt{\langle\alpha^2\rangle - \langle\alpha\rangle^2}$$

where α is the variable and $\langle\alpha\rangle$ is the expected value of α. To calculate the standard deviation, it is necessary to know the probability distribution,

$$\sigma_x = \sqrt{\int x^2|\psi(x)|^2dx - \left(\int x|\psi(x)|^2dx\right)^2} \tag{1}$$

$$\sigma_p = \sqrt{-\hbar^2\int \psi^*(x)\frac{\partial^2}{\partial x^2}\psi(x)dx - \left(i\hbar\int \psi^*(x)\frac{\partial}{\partial x}\psi(x)dx\right)^2} \tag{2}$$

4.2. Uncertainty calculation

4.2.1. Position

$$\langle x^2\rangle = \int x^2|\psi(x)|^2dx = \int_{-2}^{2} x^2\left[\frac{1}{2}\cos^2\left(n\frac{\pi}{4}x\right)\right]dx = \frac{4}{3} + (-1)^n\frac{8}{\pi^2 n^2}$$

$$\langle x\rangle = \int x|\psi(x)|^2dx = \int_{-2}^{2} x\left[\frac{1}{2}\cos^2\left(n\frac{\pi}{4}x\right)\right]dx = 0$$

Then,

$$\sigma_x = \sqrt{\langle x^2\rangle - \langle x\rangle^2} = 2\sqrt{\frac{1}{3} + \frac{2(-1)^n}{\pi^2 n^2}}$$

4.2.2. Momentum

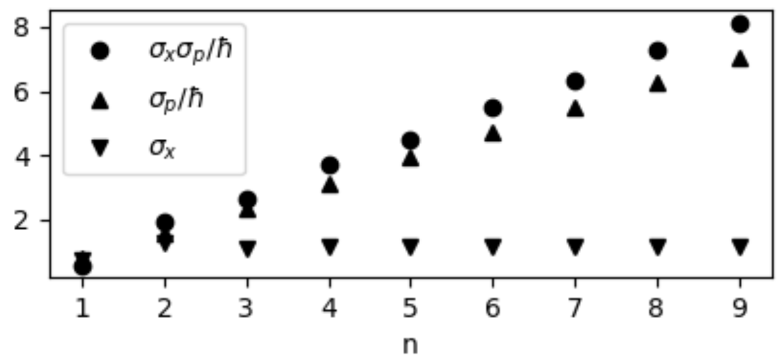
$$\langle p^2\rangle = -\hbar^2\int \psi^*(x)\frac{\partial^2}{\partial x^2}\psi(x)dx = -\hbar^2\int_{-2}^{2}\left[\frac{1}{\sqrt{2}}cos\left(n\frac{\pi}{4}x\right)\right]\frac{\partial^2}{\partial x^2}\left[\frac{1}{\sqrt{2}}cos\left(n\frac{\pi}{4}x\right)\right]dx = \frac{\hbar^2\pi^2n^2}{8}$$

$$\langle p\rangle = i\hbar\int \psi^*(x)\frac{\partial}{\partial x}\psi(x)dx = i\hbar\int_{-2}^{2}\left[\frac{1}{\sqrt{2}}cos\left(n\frac{\pi}{4}x\right)\right]\frac{\partial}{\partial x}\left[\frac{1}{\sqrt{2}}cos\left(n\frac{\pi}{4}x\right)\right]dx = 0$$

$$\sigma_p = \sqrt{\langle p^2\rangle - \langle p\rangle^2} = \frac{\hbar\pi n}{2\sqrt{2}}$$

5. Self-explanation prompts

5.1. The following figure shown the uncertainty calculated above. Explain the meaning of each one of the three figures.



5.2. The Eisenberg uncertainty principle define $\hbar/2$ as the minimal value for $\sigma_x\sigma_p$. Show that this minimum is true for the example worked above.

5.3. The uncertainty principle applies to conjugate observables, then, can be measured with zero uncertainty two quantum observables that are not conjugate (e.g., energy and momentum)?

5.4. There is another form to calculate the uncertainty of a quantum observable. If true, calculate the uncertainty and compare your results with obtained in this example.

6. References and further reading

(a) https://mattyford.com/blog/2014/1/23/the-feynman-technique-model
(b) Fourier transform duals mean that if *G(p)* is the Fourier transformation of *g(x)*, i.e. *G(p) = FT{g(x)}*, then, the Fourier transformation of *G(p)* is proportional to *g(x)*, i.e. *g(x) = c FT{G(p)}*, where *c* is a constant.
(c) https://en.wikipedia.org/wiki/Conjugate_variables

7. Python Script to calculate and plot

```python
import numpy as np
import matplotlib.pyplot as plt
from sympy import *
init_session()

x,p,hbar = symbols('x,p,hbar')
n = symbols('n', integer=True)
psi = cos(n*pi*x/4)/sqrt(2)

pretty_print(('psi(x)',psi))

E_x2 = simplify(integrate(x**2 * psi**2, (x, -2, 2)))
E_x  = simplify(integrate(x * psi**2, (x, -2, 2)))
sigma2_x = (E_x2 - E_x**2).simplify()

pretty_print(('sigma_x^2', sigma2_x))

E_p2 = simplify(-hbar**2*integrate(psi * diff(psi, x, 2), (x, -2, 2)))
E_p  = simplify(-1j*hbar*integrate(psi * diff(psi, x), (x, -2, 2)))

sigma2_p = (E_p2 - E_p**2).simplify()

pretty_print(('sigma_p^2', sigma2_p))

s2_x = sigma2_x.args[1][0].evalf()
s2_p = sigma2_p.args[1][0].evalf()

s2_p = s2_p.subs({hbar:1})  # It doew hbar = 1

sx = np.array([])
sp = np.array([])

n_eval = np.arange(1,10)

for nn in n_eval:
    sx = np.append(sx, sqrt(s2_x.subs({n:nn})))
    sp = np.append(sp, sqrt(s2_p.subs({n:nn})))

plt.plot(n_eval, sx, 'kv', label=r'$\sigma_x$')
plt.plot(n_eval, sp, 'k^', label=r'$\sigma_p/\hbar$')
plt.plot(n_eval, sx*sp, 'ko', label=r'$\sigma_x \sigma_p/\hbar$')
plt.xlabel('n')
plt.legend()
```

This Worked Example was proposed by Prof. David A. Miranda at Marsh 31, 2018