Quantum Bound States Exercise

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Exercise Background

Quantum-mechanical systems (structures, devices) can be separated into open systems and closed systems. Open systems are characterized with propagating or current carrying states. Closed (or bound) systems are described with localized wave-functions. One such system is a triangular potential well in MOS capacitors; another one is rectangular quantum well in heterostructure devices. In addition to this, every observable in Quantum Mechanics (like position, momentum, energy) is represented by an operator, the expectation values of which describes the mean or the mean-square location of the particle in either position space or momentum space. Position and momentum operators in a way are special operators because they do not commute, which in physical terms means that one cannot simultaneously determine the position and the momentum of the particle so that the concept of trajectory is ill-defined.

Exercise Objectives

You will be aware of the following items by successfully attempting the questions given in this assignment:

1. Learn how to work with the position and the momentum operators used in Quantum Mechanics.

2. Making use of the Bound States Calculation Lab will help you understand about the spatial spread of the wave-functions and the eigen energies in the well and will allow you to compare to infinite square well results.

Relevant Literature

The following references would be useful for further study:

1. D. K. Ferry, *Quantum Mechanics: An Introduction for Device Physicists and Electrical Engineers* (Institute of Physics Publishing, London, 2001).

2. D. Park, *Introduction to the Quantum Theory*, Dover Publications; (3rd edition, 2005).

3. J. Singh, *Quantum Mechanics: Fundamentals and Applications to Technology*, Wiley-VCH; 1 edition (1996).

4. P. Harrison, *Quantum Wells, Wires and Dots: Theoretical and Computational Physics of Semiconductor Nanostructures*, Wiley; 3rd edition (2010).

Exercise: <u>Quantum Bound States</u>

1a) We have a particle confined in a potential well given by

$$V(x) = \begin{cases} 0 & -L/2 < x < L/2 \\ \infty & 0 \end{cases}$$

Find the eigenstates and its corresponding eigenenergies

1b) Calculate the expectation value of the position operator x for the ground state. Does this correspond to the most likely location of the particle? Repeat this for state n=2.

1c) Calculate the expectation value for the momentum operator p, for the ground state. How about the expectation value for n>1? Comment on your answers whether they are classically intuitive.

1d) Compute the expectation value of x^2 and p^2 for the ground state. Work out the standard deviation of x and p, σ_x and σ_p respectively i.e.:

$$\sigma_x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$$

What is the product of their standard deviation? State the Heisenberg uncertainty principle.

1e) The Bound States Calculation Lab https://nanohub.org/tools/bsclab/ enables the simulation of the eigenstates in a finite barrier height, square quantum well. Set the quantum well width to 30nm and the well depth to 1eV and compute the eigenstates.

A. Comment on the penetration of the various wave functions into the barrier material by zooming in into the appropriate spatial region and provide plots.

B. Compare the eigenenergies computed numerically to an analytical solution obtained with the equations of 1a). Comment on differences in the eigen-energies.

C. Can you determine the equivalent infinite square well thickness for state number 1, 10, and 15?