

## Training in educational tools: Development of a toolkit for teaching quantum mechanics

**Scientific field:** Quantum physics, teaching, engineering sciences, numerical calculations

**Key words:** quantum mechanics, python, computer-simulated experiments, teaching, website, pedagogical toolkit, numerical environment

**Collaborations:** Pr. V. Kokoouline at *University of Central Florida, Orlando, USA.*

**Salary:** 600 €/month

**Period:** from September 2023 for 6 months

### Subject

*Quantum Mechanics (QM)* is responsible for the technological advances that make modern life possible such as Scanning Tunneling Microscope (STM), transistors, Blue-ray, computers, etc. QM is also at basis of new technological advances such as quantum computers, artificial intelligence, security online and so on. To supports these advances, one needs to form students and engineers with a good background in QM. However, difficulty in teaching undergraduate QM is in the counter-intuitive nature of quantum laws. Also, designing labs for a course of QM is expensive and not always possible. Our idea is to integrate experiential learning in QM classes under the form of computer-simulated experiments. For this purpose, we developed an initial version of a complete course of undergraduate QM based on numerical experiments. This framework consists on a digital learning (pedagogical tool) environment that combines (i) a series of PYTHON numerical codes and (ii) a graphical interface (see screenshot of the graphical interface in figure 1) allowing students to prepare numerical experiments demonstrating all concepts of QM, usually covered in a formal mathematical approach.

**The objective** of this proposed project is to carry on the development of the pedagogical tool to be used at Centralesupélec (CS) and the University of Central Florida (UCF). First tests were performed last year in Quantum mechanics and Statistics course given by Prof. Jean-Michel Gillet to 1A students and with students of the University of Central Florida in the context of Prof. Kokoouline's lecture in fall 2020. The candidates would take part of this project for performing the following developments:

- a) Text on the graphical interface
- b) Short lectures covering theoretical aspects of the QM concepts,
- c) In-class activities and laboratory assignments with and without the learning environment
- d) Homework assignments
- e) Some missing codes should still be developed.
- f) Integrate the developed tool with
  - i. LMS (Learning Management System) giving the possibility for the students to submit directly results of their experiential work (lab reports).
  - ii. A quantum chemistry packages (Molpro/Gaussian) for visualizing atomic/molecular orbitals and understanding the nature of the bonds (covalent/ionic) in a molecule.

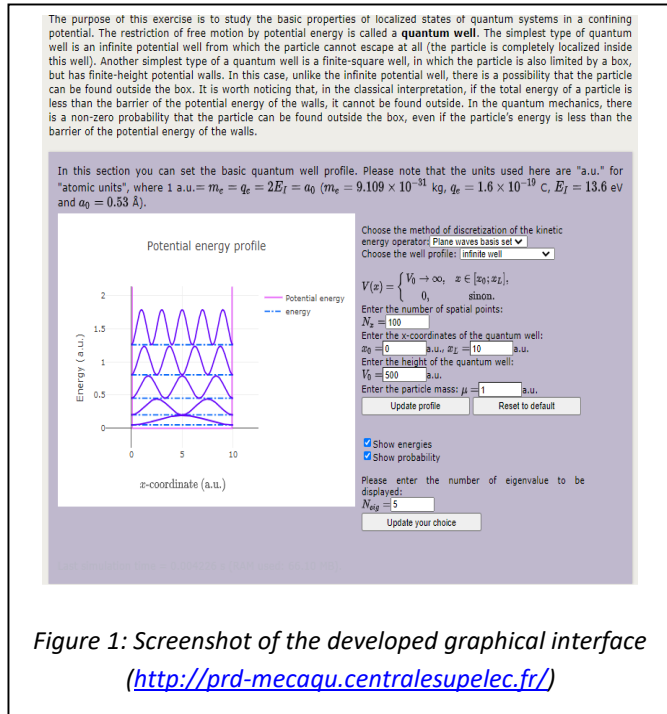


Figure 1: Screenshot of the developed graphical interface (<http://prd-mecaqu.centralesupelec.fr/>)



The candidate could choose the suitable task on which he wants to be involved, according to his/her motivation, interest and skills. The project will be conducted in collaboration with department of physics in CS and UCF.

### **Tools**

Graphical interface (see Figure 1) and Python codes dealing with the core concepts of quantum mechanics. QM standard textbooks. Find below, the employed tools to build the graphical interface: CGI: Computer-generated imagery. It is a computer graphics application to create images. NGINX: a web server used as a reverse mail proxy and HTTP cache. AJAX: Asynchronous JavaScript + XML programming languages used to create web applications.

JSON: is an open-standard file and data interchange format that uses human-readable text to transmit data objects consisting of attribute-value pairs and array data types. js - JavaScript: a high-level programming language used for web applications.

**Once again, it is not mandatory that the candidate has to master the above tools. The project could be adapted according to his/her motivation, interest and skills.**

*Collaboration with the University of Central Florida with a possibility of stay is planned for this project*

### **Responsible, co-encadrant éventuel :**

Mehdi Ayouz : [mehdi.ayouz@centralesupelec.fr](mailto:mehdi.ayouz@centralesupelec.fr)

Phone : 01 31 75 66 03 (LGPM)