Computer Simulations in Quantum Physics

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***Abstract* –** In this contribution we present our experience in using computer simulations in teaching Quantum Physics for Engineering in the Higher Technical School of Industrial Engineering in the Polytechnic University of Valencia (PUV) Valencia, Spain. We present our own code to simulate the dynamics of the one dimensional time-dependent Schrödinger equation, developed in the frame of an educational project supported by the *Instituto de Ciencias de la Educación* of our university. This software can be used by students to help them visualize and understand different quantum phenomena.

***Index terms* –** Engineering , New Technologies, Quantum-Physics, University

INTRODUCTION

For some years, the use of computational techniques to solve numerical problems in Science (and in Quantum Physics in particular) has increased considerably [1]. Thus, the efficiency in evaluating complex calculations in Physics or Engineering is much higher now than ever because of the use of computers. In fact, the computer has currently become an essential component in teaching. In what follows we will see how the use of New Technologies is included in the classroom (paying special attention to Quantum Physics for Engineering - QPE -).

QPE is a subject recently included in the studies program of the Higher Technical School of Industrial Engineering (just in 2001). In fact, we want to point out that it is the first time that this subject matter has been offered in this school.

Next, we show the main contents of the subject [2-4]:

Main contents

1.- The limits of classical Physics.
2.- Quantum radiation and matter.
    Black body radiation.
    Photoelectric effect.
    Compton effect.
    De Broglie radiation.
3.- Uncertainty relations.
    Gaussian wave packet.
    Energy-time uncertainty relation.
4.- The Schrödinger equation.
    Expectation values.
    Momentum operator.
    The expansion postulate.
5.- Time-Independent Schrödinger equation. One-dimensional potentials.
    Free particle.
    Potential step. Reflection and transmission coefficients.
    The potential barrier.
    Potential well and bound states.
    Harmonic Oscillator potential.

The delta potential.
The Kronig-Penney model.

6.- Three-dimensional problems.
Invariance under rotations.
Separation of angular momentum.
Radial equation.

7.- Hydrogen-like atom.
Separation of center-of-mass motion.
Quantum numbers.

8.- Interaction of electrons with electromagnetic field. Spin.

EDUCATIONAL FRAME

QPE is a subject offered in our school with the support of educational programs promoted by the *Instituto de Ciencias de la Educación* (ICE). These programs allow the development of tasks for the improvement of teaching and also allow the offering of fellowships to incorporate students from the university to help in educational projects. In this way, QPE is enjoying a grant devoted to giving support to teaching activities, focusing on the improvement of the basic textbook used by students (stressing the incorporation of the results of virtual simulations dealing with quantum phenomena in the book).

TEACHING QUANTUM PHYSICS FOR ENGINEERING

This way of teaching QPE allows the students to face specific quantum phenomena from different points of view. We try to be consistent when teaching different concepts (when possible) including the presentation of the theory, the resolution of selected problems, the visualization of virtual simulations and videos, and the design and implementation of the experimental work. For instance, when we deal with the photoelectric effect, the students listen to the lecturer's explanation in class; then they face how to solve proposed problems with the continual help of the professors; next, they watch virtual simulations of this effect (whether taken from Internet web sites or developed by our group). In fact, we show in this paper some of the results obtained from our own code to study one-dimensional time-dependent Schrödinger equation. This software is used with educational aims in teaching QPE. Later, the alumni watch educational videos related to the effect, and finally, they perform an experiment in the laboratory.

Any of the five different ways shown allows the student to have enough information to understand the photoelectric effect. We would like to emphasize there exists different approaches to each phenomena so that the student has no doubt in the concept analyzed. Additionally, students can ask for help during the professor's tutorial timetable to resolve any doubts the student might have. This completes the training the student receives from the educational staff.

Next, we present, as an example, the fundamentals of a code developed by our group in order to show the students some quantum phenomena with the aid of computers. We also present the results of a simulation of a wave packet evolution scattering with different one-dimensional potentials.

TIME-DEPENDENT SCHRÖDINGER EQUATION

In this work we solve the time-dependent Schrödinger equation [5] using finite difference methods [6]. The code is general enough to allow the user to study the evolution of a wave packet interacting with different potentials. In this section, and as an example, we consider a Gaussian wave packet in an initial state defined by:

$$\Psi(x,t=0) = N \cdot e^{ik_0 x} \cdot e^{-\frac{(x-x_0)^2}{\sigma^2}} \tag{1}$$

where Ψ represents the wave packet. The variables x, t represent the position and time, respectively, for which the value of the wave packet is calculated. The constants N, k_0, x_0 and σ represent a normalization constant, the central momentum of the packet, its initial position and its initial width, respectively.

The Time-dependent Schrödinger Equation takes the form:

$$-\frac{\hbar^2}{2m}\cdot\frac{\partial^2}{\partial x^2}\Psi(x,t) + V(x)\cdot\Psi(x,t) = i\hbar\frac{\partial}{\partial t}\Psi(x,t) \tag{2}$$

Our code works with the dimensionless time-dependent Schrödinger equation which is obtained making use of new variables, x’ and t’, that we define as follows:

$$t' = \frac{m \cdot c^2}{2 \cdot \hbar} t \qquad\qquad x' = \frac{m \cdot c}{\hbar} x \tag{3}$$

where x and t are the variables with their respective dimensions (space and time). These new variables yield to the next results:

$$V'(x',t') = \frac{2}{m \cdot c^2} V(x',t') \qquad\qquad E' = \frac{2}{m \cdot c^2} E \tag{4}$$

Once these new variables are defined, the dimensionless time-dependent Schrödinger equation takes the following form:

$$\left(-\frac{\partial^2}{\partial x'^2} + V(x') \right) \cdot \Psi(x',t') = i \cdot \frac{\partial \Psi(x',t')}{\partial t'} \tag{5}$$

Notice that (2) and (5) are exactly the same expressions just making the substitutions:

$$2 \cdot m \Leftrightarrow 1 \qquad\qquad \hbar \Leftrightarrow 1 \tag{6}$$

Next we show briefly the implicit finite difference scheme [3] for solving (5) for an infinite one-dimensional box potential (only as an example). We approximate $\delta^2\Psi/\delta x^2(x_i,t_{j+1})$ by the central difference approximation and $\delta\Psi/\delta t(x_i,t_{j+1})$ by the backward difference approximation to give:

$$-i \cdot \left(\frac{\Psi_{i-1,j+1} - 2 \cdot \Psi_{i,j+1} + \Psi_{i+1,j+1}}{dx^2} \right) = \left(\frac{-\Psi_{i.j} + \Psi_{i,j+1}}{dt} \right) \tag{7}$$

$\Psi_{i,j}$ being the numerical approximation to the value of $\Psi(x_i,t_j)$ and x_i, t_j the discretization nodes (dx and dt are the spatial and time steps in the discretization process).

This scheme yields to a linear system of equations for $\Psi_{i,j}$ to get the results at each time step. Thus, we have as many linear system of equations to solve as time steps. So, this is an implicit method since we must solve a linear system of equations to obtain the value of the function for each time step [6].

Solving the calculation scheme proposed in (7) we obtain solutions as the presented in figure 1.

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FIGURES AND TABLES

FIGURE 1.
WAVE FUNCTION IN AN INFINITE ONE DIMENSIONAL BOX (ARBITRARY UNITS).