

# A versatile applet to explore the wave behaviour of particles

**J I Fernández Palop**

Departamento de Física, Campus Univ. de Rabanales, Ed. C2, Planta Baja, Universidad de Córdoba, E-14071 Córdoba, Spain

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## Abstract

A pedagogical tool that consists of a Java applet has been developed so that undergraduate students in physics can explore the wave behaviour of particles. The applet executes a simulation in which a two-dimensional wave packet moves towards a slit and an obstacle with variable widths. By changing three parameters, slit width, obstacle width and initial position of the wave packet, different behaviour can be explored such as interference, diffraction produced by a slit, a corner and an obstacle, and bouncing of the wave packet, etc. The usefulness of the applet has been tested in the subject of quantum physics.

## 1. Introduction

Nowadays, there is increasing interest in developing pedagogical tools that allow a deeper learning of the subject that is being taught [1–5]. This is specially important in abstract subjects such as quantum physics [6]. When undergraduate students in physics study quantum physics for the first time, it is very difficult for them to ‘see’ how a particle can behave like a wave.

One of the first difficult concepts about wave–particle duality which a student has to learn is the uncertainty principle. An easy way to introduce this concept is to analyse the diffraction of a beam of particles through a single slit [7–9]. The distribution of particles in the screen that detects the diffraction pattern can be explained by considering the wave nature of particles. However, many times students misunderstand the diffraction and consider that it is a collective behaviour of the beam rather than being a phenomenon suffered by each single particle.

To improve the learning of the wave behaviour of particles, an applet<sup>1</sup>, programmed in Java using the Easy Java Simulations package [10–12], has been developed so that students can explore the different wave behaviour of particles. The applet implements a simulation in which a two-dimensional wave packet moves towards two objects: a slit and an obstacle, both with variable widths. The applet allows us to change three parameters for the simulation, which are the slit width, the obstacle width and the initial position of the wave packet. By

<sup>1</sup> <http://www.uco.es/hbarra/index.php/fc/appletsfc/183-schrodinger-2d-english>.

changing these parameters we can explore different behaviour of the wave packet, such as interference, diffraction produced by a slit, a corner and an obstacle, and bouncing of the wave packet, etc.

In the following sections, we will analyse the simulation, the applet and the results obtained by testing the applet with students of quantum physics.

## 2. The simulation

One of the fundamental characteristics for the applet to be useful is that the simulation must be fast so that the student can explore the wave packet evolution without wasting too much time. For this reason, the simulation takes place in a small two-dimensional  $100 \times 100$  grid. However, for the simulation to have an appreciable size, it will be shown in a  $300 \times 300$  plot.

We will use natural units, so that  $\hbar = 1$ , a particle mass  $m = 1$ , energy  $E = 1/2$  and thus momentum  $p = 1$ . The wave packet is initially centred at  $x_0 = 25$  and  $y_0 = 50$  (the unit length is given by the distance between the two consecutive points of the simulation), and thus the real and imaginary parts of the initial wave packet are given by the following vectors:

$$\begin{aligned}\psi_0^R[i][j] &= e^{-[(i-x_0)^2+(j-y_0)^2]/a^2} \cos(p \cdot i), \\ \psi_0^I[i][j] &= e^{-[(i-x_0)^2+(j-y_0)^2]/a^2} \sin(p \cdot i),\end{aligned}$$

where  $i, j = 0, \dots, 99$  and  $a = \sqrt{200}$  is the approximate width of the wave packet.

We consider a complex potential [13]. The real part of the potential is null everywhere except in the regions that define the slit or the obstacle. In these regions, where we do not want the wave packet to penetrate, the potential is thrice the energy  $E$ . The imaginary part of the potential is also null everywhere except near the walls ( $i = 0, j = 0, i = 99$  and  $j = 99$ ). In the surroundings of the walls, the imaginary part of the potential becomes gradually negative so that the wave packet is absorbed when it approaches the walls [13]. The real and imaginary parts of the potential are stored into two vectors,  $V^R[i][j]$  and  $V^I[i][j]$ , respectively.

To simulate the temporal evolution of the wave packet, we use the simplest algorithm in order to obtain a fast simulation. This algorithm consists of a direct discretization of the Schrödinger wave equation. The real and imaginary parts of the wavefunction at  $t + \Delta t$  are obtained from those at  $t$  as follows:

$$\begin{aligned}\psi_1^R[i][j] &= \psi_0^R[i][j] - \frac{\Delta t}{2\Delta x^2} (\psi_0^I[i+1][j] - 2 \cdot \psi_0^I[i][j] + \psi_0^I[i-1][j]) \\ &\quad - \frac{\Delta t}{2\Delta x^2} (\psi_0^I[i][j+1] - 2 \cdot \psi_0^I[i][j] + \psi_0^I[i][j-1]) \\ &\quad + \Delta t V^R[i][j] \psi_0^I[i][j] + \Delta t V^I[i][j] \psi_0^R[i][j], \\ \psi_1^I[i][j] &= \psi_0^I[i][j] + \frac{\Delta t}{2\Delta x^2} (\psi_0^R[i+1][j] - 2 \cdot \psi_0^R[i][j] + \psi_0^R[i-1][j]) \\ &\quad + \frac{\Delta t}{2\Delta x^2} (\psi_0^R[i][j+1] - 2 \cdot \psi_0^R[i][j] + \psi_0^R[i][j-1]) \\ &\quad - \Delta t V^R[i][j] \psi_0^I[i][j] + \Delta t V^I[i][j] \psi_0^I[i][j],\end{aligned}$$

where  $\Delta x = 1$  is the spatial discretization parameter and  $\Delta t = 0.005$  is the temporal one. The result is shown after every 100 iterations. Since this algorithm is highly unstable, the simulation is stopped after 15 000 iterations.

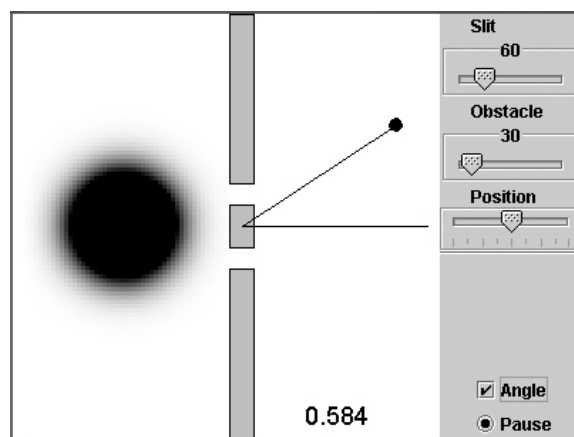


Figure 1. Window of the Java applet.

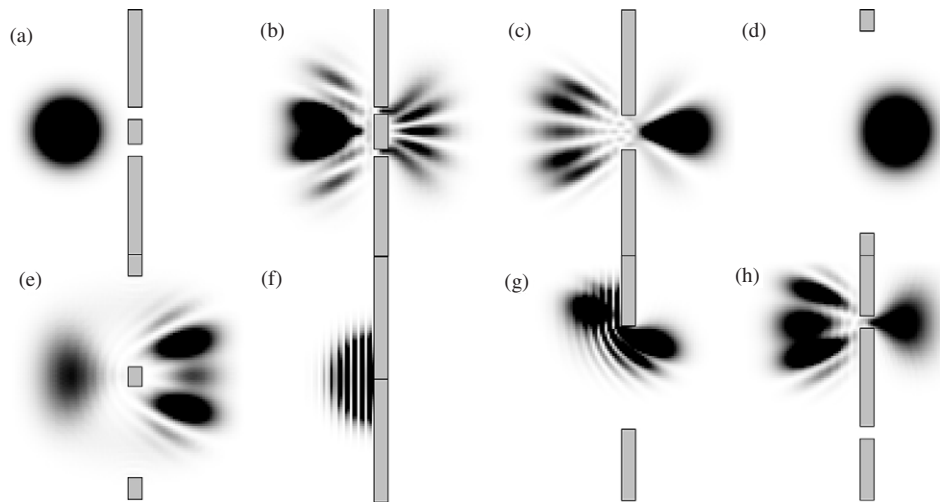
### 3. The applet

The applet has been programmed by using the package Easy Java Simulations, developed by Esquembre *et al* [10–12]. Figure 1 shows the window of the applet, which is divided into two regions. The left region contains the plot of the simulation, while the right region contains the controls to change the parameters of the simulation. There are three parameters, which are the width of the slit, labelled as ‘Slit’; the width of the obstacle, labelled as ‘Obstacle’; and the vertical position of the initial wave packet, labelled as ‘Position’. Besides, there are two buttons: one labelled as ‘Pause’, which allows us to pause the simulation, and another one labelled as ‘Angle’, which allows us to show an angle in the region of the simulation, which can be used to measure the aperture of the wave packet once it has passed through the slit and/or obstacle.

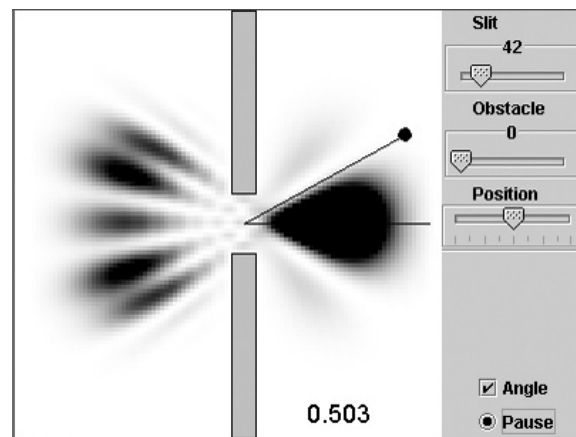
By changing the three controls, we can simulate several phenomena which are shown in figure 2. Figure 2(a) shows the initial conditions the user sees when the applet is open. The most immediate phenomena which can be observed are interference by two slits and diffraction by a single slit, which are shown in figures 2(b) and (c) respectively. Other phenomena are the free particle motion (figure 2(d)), the diffraction by an obstacle (figure 2(e)), bouncing of the particle in a wall (figure 2(f)), diffraction by a corner (figure 2(g)) and the case of two slits without interference shown in figure 2(h), due to the fact that the particle cannot ‘see’ the second slit.

The applet not only allows the qualitative exploration of different wave behaviour of particles but also provides tools to evaluate a quantitative estimation of the wavelength of the particle. Figure 3 shows the diffraction of the wave packet through a slit of width 42. The angle,  $\alpha$ , of the direction which gives the first destructive interference is related to the slit width,  $L$ , and the wavelength,  $\lambda$ , by the well-known formula  $L \sin \alpha = \lambda$  [7–9]. Figure 3 shows that  $\alpha = 0.503$ , which gives an estimative value of the wavelength  $\lambda \simeq 20.2$ . According to the parameters of the simulation, since  $p = 1$ , the wavelength of the wave packet is  $\lambda = 2\pi \times 3 = 18.85 \dots$ , where the factor 3 comes from the fact that the simulation is shown in a grid with a side thrice that of the mathematical simulation.

The applet also allows us to measure distances, since by clicking in the region of the simulation the actual position of the cursor is shown. This feature can be used to measure an estimation of the wavelength from the bouncing of the wave packet. Figure 4 shows



**Figure 2.** Different simulations which can be observed with the applet: (a) initial conditions, (b) interference, (c) diffraction by a slit, (d) free particle, (e) diffraction by an obstacle, (f) bouncing, (g) diffraction by a corner and (h) two slits without interference, since the particle cannot ‘see’ the second slit.

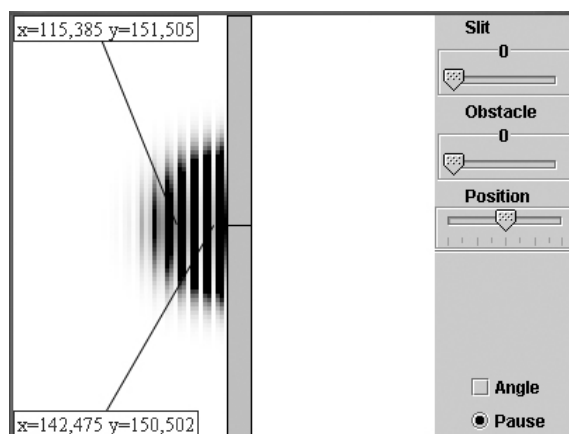


**Figure 3.** Diffraction by a slit allowing the estimation of the wavelength of the wave packet.

the bouncing just when part of the wave packet interferes with the part of the wave packet reflected by the wall. We can see dark and bright fringes due to this interference. As can be deduced from the data in figure 4, the distance among four consecutive bright fringes is  $142.475 - 115.385 = 27.09$ . Therefore, the distance between two consecutive bright fringes is 9.03, which is also equal to half the wavelength. Therefore, the wavelength can be estimated as  $\lambda \simeq 18.06$ , which is close to the correct value  $\lambda = 18.85 \dots$

#### 4. Results

The usefulness of the applet has been checked with students of quantum physics during one of the classes. This subject is studied during the third course and is compulsory to obtain a graduate level in physics.



**Figure 4.** Bouncing of the wave packet allowing us to make an estimation of the wavelength.

**Table 1.** Table given to the students.

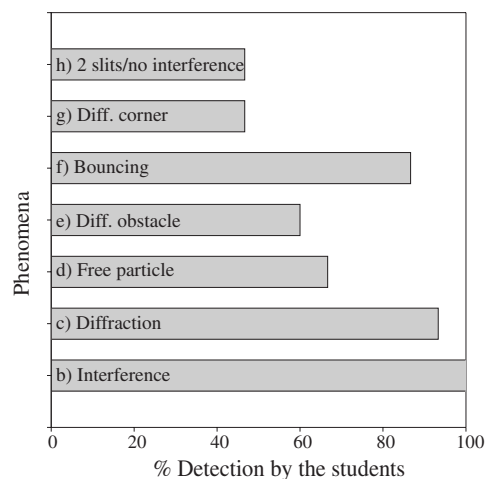
Phenomenon	Slit	Obstacle	Position
...	...	...	...

First, the applet was introduced to the students as an open problem in which they had to find as many different phenomena as possible, by changing the three controls: slit, obstacle and position. A table (table 1) was given to the students to record the results obtained. In the first column of the table, the students had to describe the concrete phenomenon they observe. In the rest of the columns, they had to write the conditions in which they observed that phenomenon, so that the teacher could reproduce the conditions and verify the observation of the student.

Afterwards, the students were asked to find different methods to measure the wavelength of the wave packet.

The results of the analysis table are shown in figure 5. Although only 20% of the students were able to find the seven phenomena shown in figure 2, the global results are good enough. Interference was found by all the students since the initial conditions of the applet show this phenomenon. Diffraction by one slit was also discovered by almost all the students, since this phenomenon is analysed during the classes in order to study Heisenberg's uncertainty principle. An interesting result is that most students included the case of a free particle, so they understand that the fact that nothing happens to the wave packet is also a different phenomenon. Another interesting result is that most students also included the case of a bounce of the wave packet, but only 20% referred to this phenomenon as a bounce, while the rest of the students referred to it as a reflection or total reflection. Around half of the students did not include these phenomena, which are usually studied in more detail in optics, such as diffraction by an obstacle or a corner. Finally, around half of the students did not include the case of two slits without interference as a different phenomenon.

With respect to the measurement of the wavelength, most students proposed the interference and/or diffraction phenomena as those suitable for measuring the wavelength. However, no one proposed the bouncing of the wave packet as suitable for measuring the wavelength. The reason consists in the fact that since the applet provides an option to measure



**Figure 5.** Results of the test, representing for each phenomenon the number of students (in %) who detected the phenomenon by using the applet.

angles, this option has to be used to measure the wavelength. However, there is no option to measure distances, although they can be measured as has been described before.

Finally, all the students found the applet to be a suitable tool to understand and explore the wave behaviour of particles.

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