Quantum mechanical phenomena are presented using visualizations based on algorithms implemented in the Interactive Data Language (IDL). A library of utilities has been written and documented. Details of the documentation, code, and how to obtain both are described below. The examples in this presentation include a simple analog of a well-known dynamic system (the bouncing ball), a technologically relevant system (electric current in a conductor), and a system that illustrates the fundamental mystery of quantum mechanics (the two-slit interference experiment). In all cases, extensive use is made of the numerical and visualization tools in IDL.

The NIST Center for Neutron Research

The NIST Center for Neutron Research (NCNR) is a national user facility providing neutron measurement capabilities to the scientific community. A robust education and outreach program helps to broaden the impact of the facility and attract new users. As part of this program, the NCNR provides summer schools and tutorials on the techniques of neutron scattering applied to condensed matter and materials research, chemistry, biology, engineering, and fundamental physics. Regardless of educational background, it is important for students to obtain an understanding of the particle-like and wave-like properties of the neutron in order to understand the fundamentals of neutron scattering. The summer school attendees come from different backgrounds, and some may not have taken a course in quantum mechanics. Therefore, it is important to provide them with an accompanying primer on the wave properties of matter. There is not enough time to provide a comprehensive mathematical introduction to quantum mechanics in a summer school or tutorial so illustrating quantum mechanical phenomena through static and dynamic visualizations can be very useful in this context.

Challenging views of visualization of quantum phenomena

In order to obtain a consistent account of atomic phenomena, it was necessary to renounce even more the use of pictures.

Niels Bohr (1955)

What Schrödinger writes about visualization scarcely makes any sense...

Werner Heisenberg (1926)

Things on a very small scale behave like nothing that you have any direct experience about. They do not behave like clouds, or billiard balls, or weights on springs, or like anything that you have ever seen. The quantum behavior of atomic objects (electrons, protons, neutrons, photons, and so on) is the same for all, they are all "particle waves," or whatever you want to call them.

Richard Feynman (1965)

Waves or particles?

Classical physics treats objects, including atomic size objects and smaller, as particles. Experiments have shown that this description of matter is incomplete. Whether the object exhibits wave-like or particle-like properties depends on the experimental details and the object’s size. In forming a microscopic picture, the quantum mechanical equation of motion—the Schrödinger equation—is solved and the results may be visualized. A way to incorporate both the particle-like and wave-like properties of an object is by modeling the object as a wave packet or pulse of waves. A wave packet has finite extent like a particle but its oscillations provide the observed wave-like properties such as interference. By using a computer to solve the Schrödinger equation and visualize the results, one can start to develop a conceptual understanding of quantum phenomena. Animated films illustrating "the time-development of quantum phenomena" were described in an important paper from 1967.

Seeing quantum interactions for the first time


In the paper referenced above, the authors present an algorithm to solve the one-dimensional time-dependent Schrödinger equation, the equation of motion that describes the dynamics of atomic-scale objects. In particular, it is applied to Gaussian wave packets representing quantum objects interacting with different environments. The value of this work was that it allowed students to "see" the time-development of quantum interactions in great detail for the first time.

The movies were recorded in a novel manner providing unique and rich windows on the quantum world but the technique was new and computers were...well...slow. In 1969, calculating the dynamics of a one-dimensional system took about 10 minutes. In 1982, the computation time was reduced to about 3-4 minutes (including graphics display) which did not permit a truly "interactive" session allowing students to explore. By 1994, the animated sequences were displayed at a frame rate of about 0.5 Hz. With the power of today’s laptops, modest graphics cards, and high-level programming languages like IDL, a truly interactive real-time experience for the student is easily attainable and straightforward to program.

The remainder of this presentation provides a few examples of quantum phenomena that can be explored today with a common laptop computer and IDL.

Obtaining the software and documentation

- Documentation (PDF book draft) contains the algorithms, descriptions, and IDL code for solving the time-dependent Schrödinger equation in one and two dimensions.
- Includes code that produces animation of quantum dynamical phenomena including scattering and transitions.
- Documentation and software is available from [http://www.ncnr.nist.gov/staff/dimeo/qvis/qvis_index.html](http://www.ncnr.nist.gov/staff/dimeo/qvis/qvis_index.html)
- The code was written to create visual demonstrations of quantum phenomena to non-experts (though the documentation is not geared towards non-experts).

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The use of certain trade names or commercial products does not imply any endorsement of a particular product, nor does it imply that the named product is necessarily the best product for the stated purpose.
We are all familiar with the motion of a bouncing ball. When dropped, it accelerates due to gravity, rebounds from the ground, and ideally rises back up to its initial height. What does that motion look like for a dropped atom, molecule, or other quantum object?

The bouncing object is modeled by a wave packet that evolves according to the quantum equation of motion. The probability of finding the particle through a direct measurement is largest where the wave packet envelope has the largest lateral extent, in the figures to the right. Note that the classical ball represented by the solid circle is often located where the lateral extent is largest. A space-time image representation of the same sequence is shown in the figure below.

Quantum features to note from these two visualizations include the spreading of the wave packet and the interference ripples during the interaction with the floor (the "bounce"). The ripples clearly seen in the frame at 5.5 ms are due to interference between rising and falling waves. A third feature to note is that the wave packet motion is not strictly periodic with the same period as the ball. The shape of the wave packet at the time at which it is dropped (t=0) is different than its shape the next time that it returns to the same position at the top of its trajectory (11.1 ms). This is related to a phenomenon known as collapse and revival of the wave packet which occurs over the course of many bounces.

The frames of a quantum object bouncing three times (sequentially ordered left to right/top to bottom) are taken at successive increments in time. The entire sequence is about 32 ms. This shows how an object with a neutron mass and an initial spatial extent 38 \(\mu\)m (full-width at half-maximum of the wave packet) would propagate in a gravitational field when dropped from a height of 150 m. The solid black circle represents the classical particle's position. The solid envelope represents the absolute value of the wave packet, the solid wiggly line within the envelope is the real part of the wave packet, and the dashed wiggly line within the envelope is the imaginary part of the wave packet.

You can find an experimental realization of this that uses neutrons in the paper: Quantum states of neutrons in the Earth’s gravitational field, Nature vol. 415, p. 297 (2002) by Valery Nesvizhevsky et. al. In that experiment, neutrons were directed horizontally into a channel composed of a reflecting mirror as the "floor" and an absorbing "ceiling." The number of neutrons were counted at the exit of this channel as a function of the separation distance between the floor and ceiling. The resulting transmission was composed of a series of steps corresponding to the interference ripples seen above.
electron propagation in a solid

In the classical picture of electrical conduction, electrons accelerate in an applied electric field and occasionally collide with atoms. The successive accelerations and collisions result in a net drift velocity of the point-like electrons. The product of the charge and their drift velocity is the electric current.

But electrons are quantum entities. So, what does electronic conduction in a metal look like quantum mechanically?

We can model the electron as a wave packet and the metal as a spatially oscillating function of positive and negative peaks that correspond to the underlying crystal lattice.

One of the unique consequences of the wave-like nature of an electron is that its propagation in a periodic structure strongly depends on (1) the velocity of the wave packet and (2) the periodic nature of the lattice. For particular values of the particle’s velocity, the wave packet cannot propagate in the structure (known as the Bragg condition). For other values of the wave packet’s velocity, the wave packet can propagate. This phenomenon of conditional propagation is a key feature of the wave nature of matter and it is also central to the theory of electrical conduction in conductors and semiconductors.

On seeing animated films of wave packet scattering in a crystal lattice for the first time in 1978 one physicist noted...

Quite aside from their pedagogic value these films are visually very beautiful, easily on par with visual displays occasionally shown in museums of modern art.

The propagation of a wave packet in a crystal proves to have the elegance and grace of the best ballet.

Kurt Gottfried
American Journal of Physics 46, 315 (1978)

A wave packet that propagates towards the periodic structure will either (1) split so that part of the wave packet penetrates and part of it reflects or (2) undergo nearly complete reflection. The former case is representative of electron transmission/reflection at a boundary. The latter case is a consequence of the Bragg condition. The electric current is related to the number of electrons that are transmitted through the potential. Since an impurity (e.g. a random variation of the lattice) will reflect some of the propagating electron wave packet, it will reduce the number of electrons transmitted and is a contributor to the electrical resistance.

The figure above illustrates propagation of a wave packet in a periodic structure when the Bragg condition is not satisfied. Note that much of the wave packet is transmitted but part of it is reflected. The physical length of each frame is about 9.8 nm and the duration of the event is about 5 femtoseconds (5x10^-15 s). Arrows indicate the propagation direction.

The figure above illustrates propagation of a wave packet in a periodic structure when the velocity of the wave packet is a value for which propagation in the structure is not supported. Therefore, most of the wave packet is reflected and only a small amount propagates into the structure. It is also interesting to note how far the wave packet propagates into the structure before reflection.

This figure illustrates propagation of a wave packet in a periodic structure with an impurity (a random change in amplitude over a small part of the lattice). With no impurity, the wave packet would propagate freely in the structure as seen in the top-most figure on this page. However, the presence of the impurity splits the wave packet into transmitted and reflected components.
Visualizing Wave-Particle Duality

The fundamental mystery of quantum mechanics has been referred to as wave-particle duality. Really small things (atomic size and smaller) sometimes behave like particles and sometimes behave like waves, depending upon the way the measurement is made. The experiment that exemplifies this peculiar behavior is the two-slit interference experiment that has been performed for light, electrons, neutrons, and atoms.

The slit system is modeled as a very high barrier over a two-dimensional region defining the extent of the slits. There is no barrier at the location of the slits. This is designed so that nothing can penetrate the non-slit regions.

Previously, we solved the one-dimensional quantum equation of motion, but it is straightforward to extend it to higher dimensions. We can easily simulate the two-slit experiment by generalizing the algorithm so that our quantum object (e.g. electron, neutron) is modeled as a two-dimensional wave packet.

We illustrate wave-particle duality using two different visualizations. In the first case, we solve the quantum equation of motion for a two-dimensional wave packet interacting with the two-slit system (upper right panel). The wave-like nature of the interaction is clear from the interference patterns that appear both to the right and to the left of the slits.

The visualization in the lower right panel illustrates the time-evolution of the signal received in a detector on the far side of the slit system. This shows how the interference pattern builds up over time as more and more quantum objects are launched towards the slit system. The pattern recorded in the simulated detector is similar to the results from measurements carried out using electrons and neutrons, for example, that have been described classically.


The sequence of frames above simulates how an experiment might proceed after a number of quantum objects scatter or transmit through the two-slit system. In the configuration above, a position-sensitive detector is placed to the right of the slit system. The number at the top of each frame represents the total number of objects launched towards the slits but only the objects that do not reflect backwards are "counted" in the detector. The individual dots to the right of the slits represent "hits" in the detector. In the early frames single hits appear at random locations on the detector screen. As the number of events increases a clear "banding" appears signifying interference, which is a hallmark of wave behavior.