Wave packet scattering in one dimension

visualizations of transmission and reflection phenomena
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RESTRICTED
SOME MATERIAL NOT SUITABLE FOR ALL AUDIENCES
CONTAINS COMPLEX MATHEMATICS, ABSTRACT PHYSICAL CONCEPTS, AND GRATUITOUS JARGON

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Reflectionless eigenstates of the sech^2 potential

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(Received 23 May 2007; accepted 28 August 2007)

The one-dimensional potential well \( V(x) = -\left(\hbar^2 \nu(\nu+1)/2ma^2\right) \text{sech}^2(x/a) \) does not reflect waves of any energy when \( \nu \) is a positive integer. We show that in this reflectionless case the solutions of Schrödinger’s equation can be expressed in terms of elementary functions. Wave packets can be constructed from these energy eigenstates, and the propagation of such wave packets through the potential region can be studied analytically. We find that the group velocity of a particular packet can substantially exceed the group velocity of a free-space Gaussian packet. The bound states of the potential can also be expressed in terms of elementary functions when \( \nu \) is an integer. The special properties of the integer \( \nu \) potentials are associated with critical binding. © 2007 American Association of Physics Teachers.

[DOI: 10.1119/1.2787015]
Visualization/conceptualization just plain weird

“Things on a very small scale behave like nothing that you have any direct experience about. They do not behave like waves, they do not behave like particles, the do not behave like clouds, or billiard balls, or weights on springs, or like anything that you have ever seen.”

Visualization/conceptualization not without controversy

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

The more I think of the physical part of the Schrödinger theory, the more detestable I find it.

What Schrödinger writes about visualization scarcely makes any sense, in other words, I think it is shit.

The greatest results of his theory is the calculation of matrix elements.

Werner Heisenberg in a letter to Wolfgang Pauli (June 8, 1926)
It is important to keep in mind that the wave packets in the ensemble are not intended to correspond to the individual neutrons in the beam. If this were so then each neutron in the beam would be in a pure state. In fact, each neutron is in a mixed state that is represented by the ensemble of wave packets...there is clearly not a one-to-one correspondence between the neutrons and the wave packets.

-neutron optics expert
Phasors

\[ \psi = \psi_{re} + i \psi_{im} \]

**Figure 8** Arrows that represent each possible way an event could happen are drawn and then combined (“added”) in the following manner. Attach the head of one arrow to the tail of another—without changing the direction of either one—and draw a “final arrow” from the tail of the first arrow to the head of the last one.
Computer-Generated Motion Pictures of One-Dimensional Quantum-Mechanical Transmission and Reflection Phenomena*

Abraham Goldberg and Harry M. Schry†
Lawrence Radiation Laboratory, University of California, Livermore, California

and

Judah L. Schwartz
Science Teaching Center, Massachusetts Institute of Technology, Cambridge, Massachusetts
(Received 4 October 1966)

We describe the details involved in presenting the time development of one-dimensional quantum-mechanical systems in the form of computer-generated motion pictures intended for pedagogic purposes. Concentrating on reflection-transmission phenomena, we formulate the problem in terms of a Gaussian wave packet impinging on a square well or barrier and being reflected and transmitted. The wave equation is solved numerically by methods discussed in detail and photographs of the wave packet vs position at a variety of times and for a range of projectile energies are given.
On the visualization of a wave packet propagating in a crystal

"Quite aside from their pedagogical 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."

Launching wavepackets at a barrier
a numerical “experiment”

Analytical

“Experimental”
Launching wavepackets at a barrier
a numerical “experiment”

Analytical

\[ r(k_o) = 1 - \int_{-\infty}^{\infty} dk \ T(k) \ P(k; k_o) \]

\[ P(k; k_o) = |\varphi(k, 0; k_o)|^2 \]

\[ \varphi(k, t = 0; k_o) = \left( \frac{\sigma_x^2}{\pi} \right)^{\frac{1}{4}} e^{-\frac{1}{2} \sigma_x^2 (k-k_o)^2} \]

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**“Experimental”**

Launch wavepackets with different \( k_o \)

Wait until the reflected wavepacket is far enough away from the barrier so that it is no longer interacting with it

“Measure” the amount reflected (integrated probability density)
Launching wavepackets at a barrier

a numerical “experiment”

Reflection probability

$V = 63170$
$w = 0.021$
$\sigma_x = 0.05$
Launching wavepackets at a structure

wavepacket width effects

Reflection probability

plane wave calculation

wave packet calculation

\( \sigma_x = 20 \)
Launching wavepackets at a structure

wavepacket width effects
Launching wavepackets at a structure

wavepacket width effects

Reflection probability

plane wave calculation

wave packet calculation

$\sigma_x = 5$

$k_o$
Launching wavepackets at a structure
wavepacket width effects
Reflection from an oscillating barrier
multi-phonon exchange

\[ E_n = E_o + n\hbar \omega \]

\[ k_n = -\sqrt{2E_n} \]

\[ dx(t) = \delta \sin \omega t \]

\[ V = (5/2) k_o^2 \]

Reflection from a stationary barrier
reminder: what does it look like?
Reflection from an oscillating barrier
what does it look like?
Reflection from an oscillating barrier
momentum distribution: $k_o^2/2 < \omega$

$k_o = 400 \Rightarrow k_n = -400, -798, -1054, -1261, -1437, ...$
Reflection from an oscillating barrier
momentum distribution: \( k_o^2/2 > \omega \)

\[ k_o = 750 \Rightarrow k_n = -294, -750, -1019, -1231, -1411, -1571, -1716, \ldots \]
BACKUP
Computer-Generated Motion Pictures of One-Dimensional Quantum-Mechanical Transmission and Reflection Phenomena*

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Solving the Schrodinger Equation
Finite-difference time-domain method

The reader will note occasional breaks or discontinuities at various points in some of these pictures. This effect is due to an evidently inherent malfunction of the equipment involved in rendering the machine calculations into graphical form. At the present time there appears to be no simple way to avoid this problem...This situation emphasizes the fact that the use of computers to illustrate time development in physical systems by motion pictures is still in a preliminary, if no longer rudimentary, stage.
Solving the Schrödinger Equation

Finite-difference time-domain method

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A fast explicit algorithm for the time-dependent Schrödinger equation

P. B. Visscher

Department of Physics and Astronomy, University of Alabama, Tuscaloosa, Alabama 35487-0324

(Received 9 November 1990; accepted 1 May 1991)

An explicit algorithm for the time-stepping solution of the Schrödinger equation is described, which is second-order accurate in time. It is a staggered-time algorithm, in which the real and imaginary parts of the wave function are defined at alternate times. The method combines the speed and simplicity of explicit methods with the accuracy and stability of second-order implicit methods. Because of this simplicity and speed, the algorithm is well suited for pedagogical applications on personal computers, as well as for computation-intensive research applications.
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P.B. Visscher, Computers in Physics, 5, 596 (1991)
Absorbing boundary conditions for the finite-difference time-domain calculation of the one-dimensional Schrödinger equation

Tsugumichi Shibata

NTT LSI Laboratories, 3-1 Morinosato Wakamiya, Atsugi 243-01, Japan
(Received 30 August 1990)

The absorbing boundary conditions for the finite-difference calculation of the time-dependent one-dimensional Schrödinger equation are presented. These are the local boundary conditions that approximate the one-way wave equation of a wave function. The conditions minimize undesirable reflections at the artificial boundaries of the area of computation, thus enabling us to limit the computation area efficiently. The calculations of the transmission coefficient of multibarrier tunneling show the validity of the method.
Absorbing boundary conditions
T. Shibata, PRB, 43, 6760 (1991)

\[ \Psi(x, t) = e^{-i(\omega t - kx)} \]

\[ i\hbar \frac{\partial}{\partial t} \Psi(x, t) = \left[ -\frac{\hbar^2}{2m^*} \frac{\partial^2}{\partial x^2} + U(x) \right] \Psi(x, t) \]
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\[ \hbar k = \pm \left[ 2m^*(\hbar \omega - U) \right]^{1/2} \]
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Quantum bouncer realized with neutrons

Nesvizhevsky et. al., Quantum states of neutrons in Earth’s gravitational field, Nature 415, 297 (2002).
Quantum bouncer realized with neutrons

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\[ v_n = 1.7 \, \text{cm/s} \]
\[ h = 14.7 \, \text{mm} \]