Enhancing the Undergraduate Physics Curriculum with Computation

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Partnership for Integration of Computation into Undergraduate Physics

PICUP

PARTNERSHIP FOR INTEGRATION OF COMPUTATION INTO UNDERGRADUATE PHYSICS

1. PICUP

- Purpose: Lower barriers for faculty across the country to integrate computation into their STEM courses
- PICUP has existed in some form for 12+ years
  * http://compphysed.shodor.org/
  * NSF-funded since 2015: www.gopicup.org
- The PICUP Collection
- for more details on the PICUP Community and Events also see recording of first webinar in this series: https://youtu.be/eXf1MXRDowg

2. How Computation Enhances Course Content in the Sciences and Engineering

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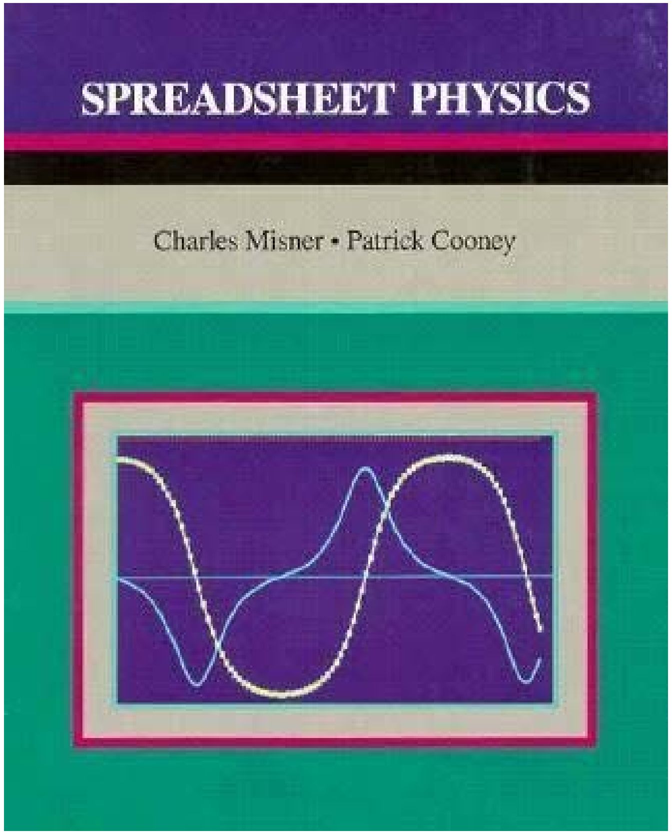
Spreadsheets-the Lost Art



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My Model for Integrating Computation

(into intro courses populated by students who have never programmed before)

- Start with Excel
- **"Guided Activities"** in Excel (I GUIDE the construction of models in Excel and students use their Excel as a GUIDE)
    - Build algorithm visually (students have a working model)
    - Investigate accuracy
    - Use model to calculate something (investigate dynamic behavior)
- Use Excel implementation as a Guide to produce MATLAB or C or Python version from scratch
- After 3 or 4 of these **"Guided Activities"**, the students code in MATLAB or C or Python from scratch w/o spreadsheet GUIDE

Computation in the Undergraduate Curriculum

* Early
* Often
* Enhances Content Coverage
* Exposes Students to More (and Interesting!), Sooner

Damped, Driven Oscillations

(from Halliday, Resnick, and Walker, 9th ed.)

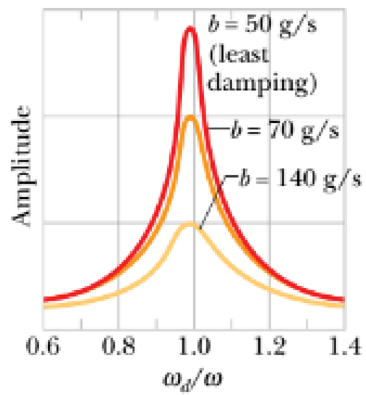


Fig. 15-16 The displacement amplitude x_m of a forced oscillator varies as the angular frequency ω_d of the driving force is varied. The curves here correspond to three values of the damping constant b.

15-9 Forced Oscillations and Resonance

A person swinging in a swing without anyone pushing it is an example of *free oscillation*. However, if someone pushes the swing periodically, the swing has *forced*, or *driven, oscillations*. *Two* angular frequencies are associated with a system undergoing driven oscillations: (1) the *natural* angular frequency ω of the system, which is the angular frequency at which it would oscillate if it were suddenly disturbed and then left to oscillate freely, and (2) the angular frequency ω_d of the external driving force causing the driven oscillations.

We can use Fig. 15-14 to represent an idealized forced simple harmonic oscillator if we allow the structure marked "rigid support" to move up and down at a variable angular frequency ω_d. Such a forced oscillator oscillates at the angular frequency ω_d of the driving force, and its displacement $x(t)$ is given by

$$x(t) = x_m \cos(\omega_d t + \phi), \qquad (15\text{-}45)$$

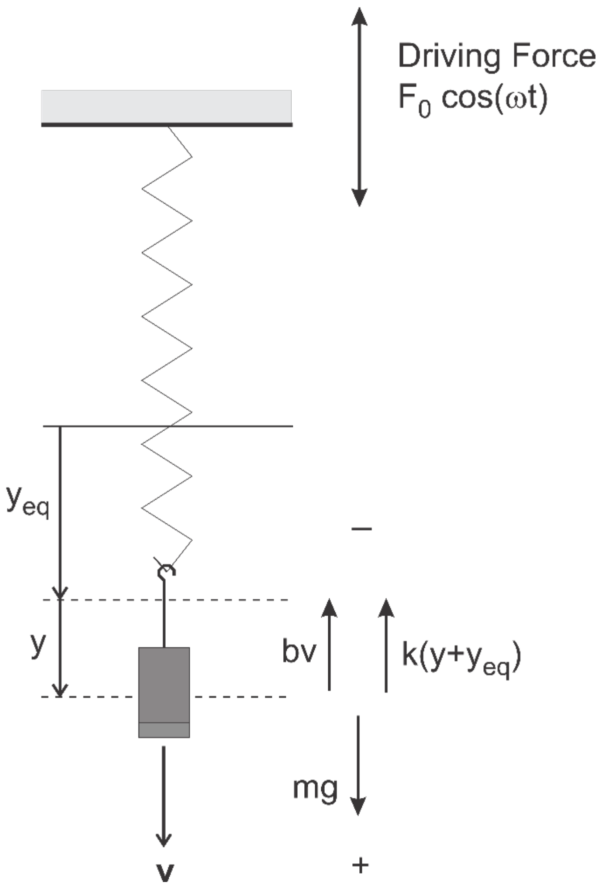
where x_m is the amplitude of the oscillations.

How large the displacement amplitude x_m is depends on a complicated function of ω_d and ω. The velocity amplitude v_m of the oscillations is easier to describe: it is greatest when

$$\omega_d = \omega \qquad \text{(resonance)}, \qquad (15\text{-}46)$$

a condition called **resonance.** Equation 15-46 is also *approximately* the condition

Hanging Spring



Newton's 2nd law:

$$\sum F = mg - bv - k\left(y + y_{eq}\right) + F_0 \cos\left(\omega t\right)$$

$$\implies \ddot{y}(t) = -\frac{k}{m} y(t) - \frac{b}{m}\dot{y}(t) + \frac{F_0}{m}\cos(\omega t).$$

Solve via Analytical Guess

\- or -

Computationally via Euler-Cromer Algorithm

$$v\left(t + \Delta t\right) \approx v\left(t\right) + a\left(t\right)\Delta t$$

$$y\left(t + \Delta t\right) \approx y\left(t\right) + v\left(t + \Delta t\right)\Delta t$$

Rocket Motion

(from Halliday, Resnick, and Walker, 9th ed.)

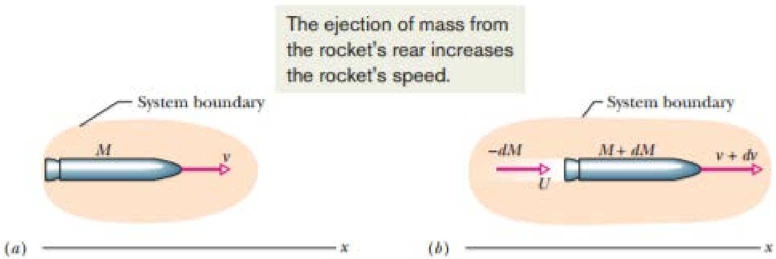


Fig. 9-22 (*a*) An accelerating rocket of mass M at time t, as seen from an inertial reference frame. (*b*) The same but at time $t + dt$. The exhaust products released during interval dt are shown.

Figure 9-22*b* shows how things stand a time interval dt later. The rocket now has velocity $v + dv$ and mass $M + dM$, where the change in mass dM is a *negative quantity*. The exhaust products released by the rocket during interval dt have mass $-dM$ and velocity U relative to our inertial reference frame.

Our system consists of the rocket and the exhaust products released during interval dt. The system is closed and isolated, so the linear momentum of the system must be conserved during dt; that is,

$$P_i = P_f, \tag{9-82}$$

where the subscripts i and f indicate the values at the beginning and end of time interval dt. We can rewrite Eq. 9-82 as

$$Mv = -dM\,U + (M + dM)(v + dv), \tag{9-83}$$

where the first term on the right is the linear momentum of the exhaust products released during interval dt and the second term is the linear momentum of the rocket at the end of interval dt.

We can simplify Eq. 9-83 by using the relative speed v_{rel} between the rocket and the exhaust products, which is related to the velocities relative to the frame with

$$\begin{pmatrix}\text{velocity of rocket}\\ \text{relative to frame}\end{pmatrix} = \begin{pmatrix}\text{velocity of rocket}\\ \text{relative to products}\end{pmatrix} + \begin{pmatrix}\text{velocity of products}\\ \text{relative to frame}\end{pmatrix}.$$

In symbols, this means

$$(v + dv) = v_{rel} + U,$$

or

$$U = v + dv - v_{rel}. \tag{9-84}$$

Substituting this result for U into Eq. 9-83 yields, with a little algebra,

$$-dM\,v_{rel} = M\,dv. \tag{9-85}$$

Dividing each side by dt gives us

$$-\frac{dM}{dt}v_{rel} = M\frac{dv}{dt}. \tag{9-86}$$

We replace dM/dt (the rate at which the rocket loses mass) by $-R$, where R is the (positive) mass rate of fuel consumption, and we recognize that dv/dt is the acceleration of the rocket. With these changes, Eq. 9-86 becomes

$$Rv_{rel} = Ma \quad \text{(first rocket equation).} \tag{9-87}$$

Equation 9-87 holds for the values at any given instant.

Note the left side of Eq. 9-87 has the dimensions of force (kg/s · m/s = kg · m/s² = N) and depends only on design characteristics of the rocket engine—namely, the rate R at which it consumes fuel mass and the speed v_{rel} with which

Rocket Motion (from Halliday, Resnick, and Walker, 9th ed.)

that mass is ejected relative to the rocket. We call this term Rv_{rel} the **thrust** of the rocket engine and represent it with T. Newton's second law emerges clearly if we write Eq. 9-87 as $T = Ma$, in which a is the acceleration of the rocket at the time that its mass is M.

Finding the Velocity

How will the velocity of a rocket change as it consumes its fuel? From Eq. 9-85 we have

$$dv = -v_{\text{rel}} \frac{dM}{M}.$$

Integrating leads to

$$\int_{v_i}^{v_f} dv = -v_{\text{rel}} \int_{M_i}^{M_f} \frac{dM}{M},$$

in which M_i is the initial mass of the rocket and M_f its final mass. Evaluating the integrals then gives

$$v_f - v_i = v_{\text{rel}} \ln \frac{M_i}{M_f} \qquad \text{(second rocket equation)} \qquad (9\text{-}88)$$

for the increase in the speed of the rocket during the change in mass from M_i to M_f. (The symbol "ln" in Eq. 9-88 means the *natural logarithm*.) We see here the advantage of multistage rockets, in which M_f is reduced by discarding successive stages when their fuel is depleted. An ideal rocket would reach its destination with only its payload remaining.

sec. 9-12 Systems with Varying Mass: A Rocket

•76 A 6090 kg space probe moving nose-first toward Jupiter at 105 m/s relative to the Sun fires its rocket engine, ejecting 80.0 kg of exhaust at a speed of 253 m/s relative to the space probe. What is the final velocity of the probe?

•77 SSM In Fig. 9-70, two long barges are moving in the same direction in still water, one with a speed of 10 km/h and the other with a speed of 20 km/h. While they are passing each other, coal is shoveled from the slower to the faster one at a rate of 1000 kg/min. How much additional force must be provided by the driving engines of (a) the faster barge and (b) the slower barge if neither is to change speed? Assume that the shoveling is always perfectly sideways and that the frictional forces between the barges and the water do not depend on the mass of the barges.

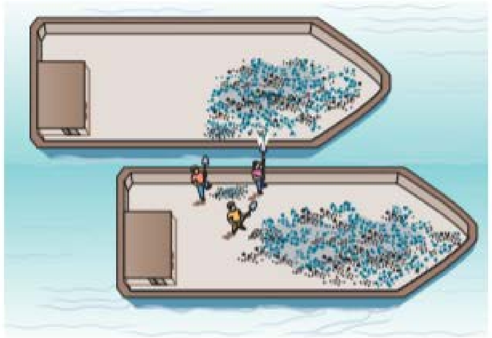
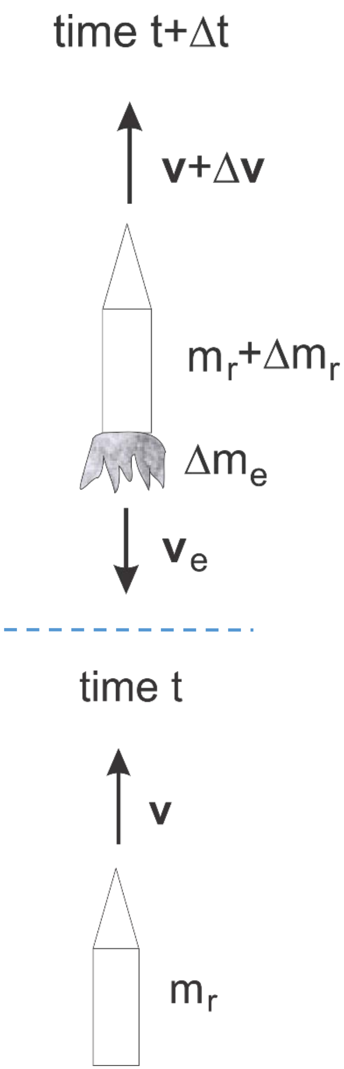


Fig. 9-70 Problem 77.

•78 Consider a rocket that is in deep space and at rest relative to an inertial reference frame. The rocket's engine is to be fired for a certain interval. What must be the rocket's *mass ratio* (ratio of initial to final mass) over that interval if the rocket's original speed relative to the inertial frame is to be equal to (a) the exhaust speed (speed of the exhaust products relative to the rocket) and (b) 2.0 times the exhaust speed?

•79 SSM ILW A rocket that is in deep space and initially at rest relative to an inertial reference frame has a mass of 2.55×10^5 kg,

Saturn V Rocket Launch



$$m_r \frac{\Delta \mathbf{v}}{\Delta t} + \frac{\Delta m_e}{\Delta t}\mathbf{v}_e \approx \sum \mathbf{F}_{ext}$$

$$\Longrightarrow \ddot{y}(t) \approx -\frac{GM_E}{[R_E + y(t)]^2} + \frac{T}{m_r(t)}$$

Very Difficult (or Impossible!) Analytically

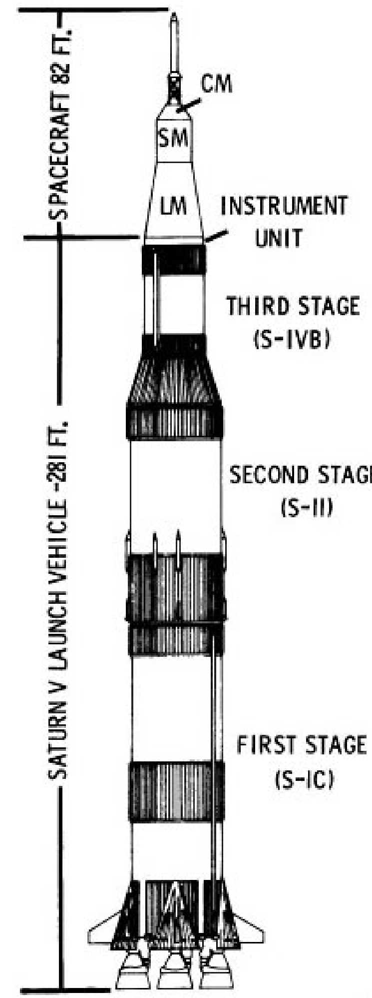
\- or -

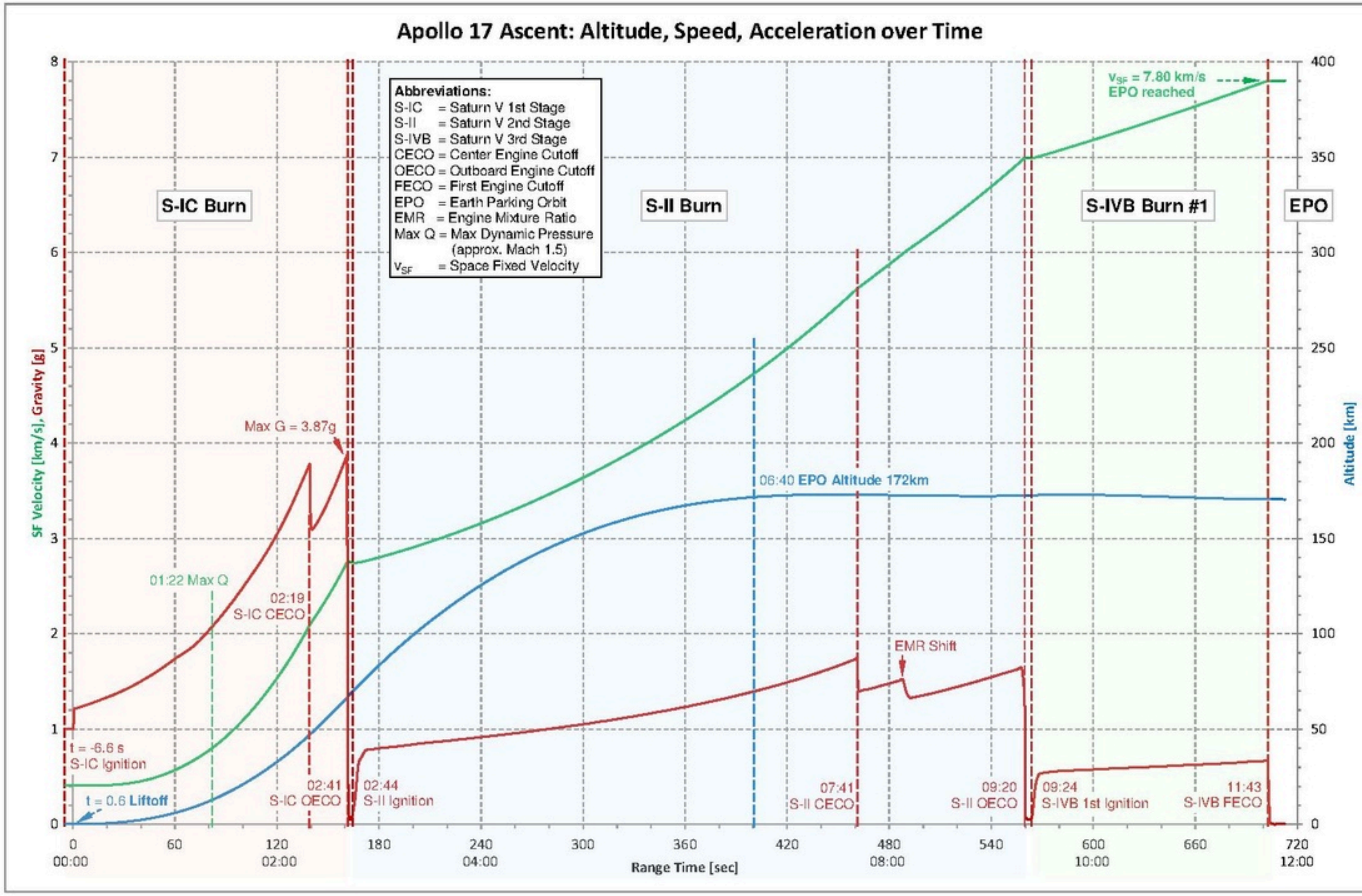
Computationally via Euler-Cromer Algorithm

$$v\left(t+\Delta t\right) \approx v\left(t\right) + a\left(t\right)\Delta t$$

$$y\left(t+\Delta t\right) \approx y\left(t\right) + v\left(t+\Delta t\right)\Delta t$$

$$m_r(t+\Delta t) = m_r(t) - \frac{T}{v_e}\Delta t,$$




Apollo 17 Ascent: Altitude, Speed, Acceleration over Time
Abbreviations:
S-IC = Saturn V 1st Stage
S-II = Saturn V 2nd Stage
S-IVB = Saturn V 3rd Stage
CECO = Center Engine Cutoff
OECO = Outboard Engine Cutoff
FECO = First Engine Cutoff
EPO = Earth Parking Orbit
EMR = Engine Mixture Ratio
Max Q = Max Dynamic Pressure (approx. Mach 1.5)
V_{SF} = Space Fixed Velocity
S-IC Burn
S-II Burn
S-IVB Burn #1
EPO
V_{SF} = 7.80 km/s
EPO reached
Max G = 3.87g
06:40 EPO Altitude 172km
01:22 Max Q
02:19
S-IC CECO
EMR Shift
t = -6.6 s
S-IC Ignition
t = 0.6 Liftoff
02:41
S-IC OECO
02:44
S-II Ignition
07:41
S-II CECO
09:20
S-II OECO
09:24
S-IVB 1st Ignition
11:43
S-IVB FECO
SF Velocity [km/s], Gravity [g]
Altitude [km]
Range Time [sec]
0
00:00
60
120
02:00
180
240
04:00
300
360
420
480
08:00
540
600
10:00
660
720
12:00

Discretization

-Physics: Schrodinger Equation
-Engineering Heat Equation, Diffusion Equation

* Explicit numerical approach is all that is needed
  - add source terms
  - more than 1D
  - transient response
  - beyond idealistic (needs to be easy for analytical approach)
  - can be doe w/o continuum limit calculus
  - mathematical preparation Taylor series

Traditional Approach to Introducing QM Scattering

1. Solve Time-INDEPENDENT Schrödinger Equation in different regions of PE

p. 66 from "Introduction to Quantum Mechanics"
by David J. Griffiths, Pearson Prentice Hall, 1995

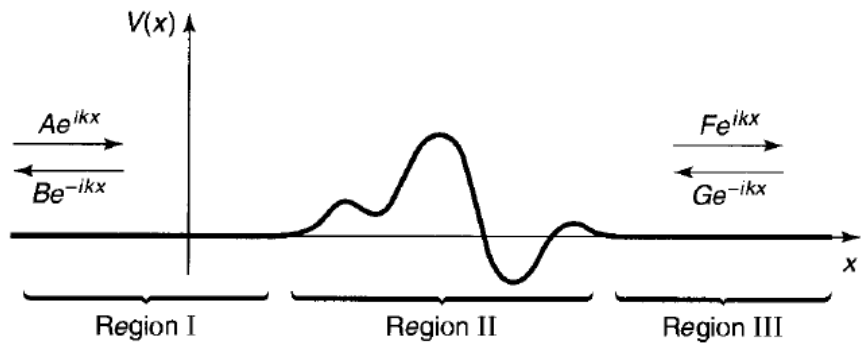


Figure 2.15: Scattering from an arbitrary localized potential [$V(x) = 0$ except in Region II].

2. Calculate R and T from:

$$R \equiv \frac{|B|^2}{|A|^2} \quad \text{and} \quad T \equiv \frac{|F|^2}{|A|^2}$$

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> [redacted]ough straightforward in principle, this is a messy business in practice, a[redacted]at this point it is best to turn the problem over to a computer.[38]

By Davi[redacted]. Griffiths, Pearson Prentice Hall, 2005

Of course, the *sum* of these probabilities should be 1—and it *is*:

$$R + T = 1. \qquad [2.140]$$

Notice that R and T are functions of β, and hence (Equations 2.130 and 2.135) of E:

$$R = \frac{1}{1 + (2\hbar^2 E/m\alpha^2)}, \quad T = \frac{1}{1 + (m\alpha^2/2\hbar^2 E)}. \qquad [2.141]$$

The higher the energy, the greater the probability of transmission (which certainly seems reasonable).

This is all very tidy, but there is a sticky matter of principle that we cannot altogether ignore: These scattering wave functions are not normalizable, so they don't actually represent possible particle states. But we know what the resolution to this problem is: We must form normalizable linear combinations of the stationary states, just as we did for the free particle—true physical particles are represented by the resulting wave packets. Though straightforward in principle, this is a messy business in practice, and at this point it is best to turn the problem over to a computer.[38] Meanwhile, since it is impossible to create a normalizable free-particle wave function without involving a *range* of energies, R and T should be interpreted as the *approximate* reflection and transmission probabilities for particles in the *vicinity* of E.

Incidentally, it might strike you as peculiar that we were able to analyze a quintessentially time-dependent problem (particle comes in, scatters off a potential, and flies off to infinity) using *stationary* states. After all, ψ (in Equations 2.131 and 2.132) is simply a complex, time-independent, sinusoidal function, extending (with constant amplitude) to infinity in both directions. And yet, by imposing appropriate boundary conditions on this function we were able to determine the probability that a particle (represented by a *localized* wave packet) would bounce off, or pass through, the potential. The mathematical miracle behind this is, I suppose, the fact that by taking linear combinations of states spread over all space, and with essentially trivial time dependence, we can *construct* wave functions that are concentrated about a (moving) point, with quite elaborate behavior in time (see Problem 2.43).

[37]This is not a normalizable wave function, so the *absolute* probability of finding the particle at a particular location is not well defined; nevertheless, the *ratio* of probabilities for the incident and reflected waves *is* meaningful. More on this in the next paragraph.

[38]Numerical studies of wave packets scattering off wells and barriers reveal extraordinarily rich structure. The classic analysis is A. Goldberg, H. M. Schey, and J. L. Schwartz, *Am. J. Phys.* **35**, 177 (1967); more recent work can be found on the Web.

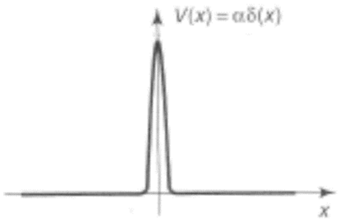

FIGURE 2.16: The delta-function barrier.

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AMERICAN JOURNAL of PHYSICS

A Journal Devoted to the Instructional and Cultural Aspects of Physical Science

VOLUME 35, NUMBER 3 MARCH 1967

Computer-Generated Motion Pictures of One-Dimensional Quantum-Mechanical Transmission and Reflection Phenomena*

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(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.

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A. Goldberg, H.M. Schey, and J.L. Schwartz, Am. J. Phys. **35**, 177 (1967)

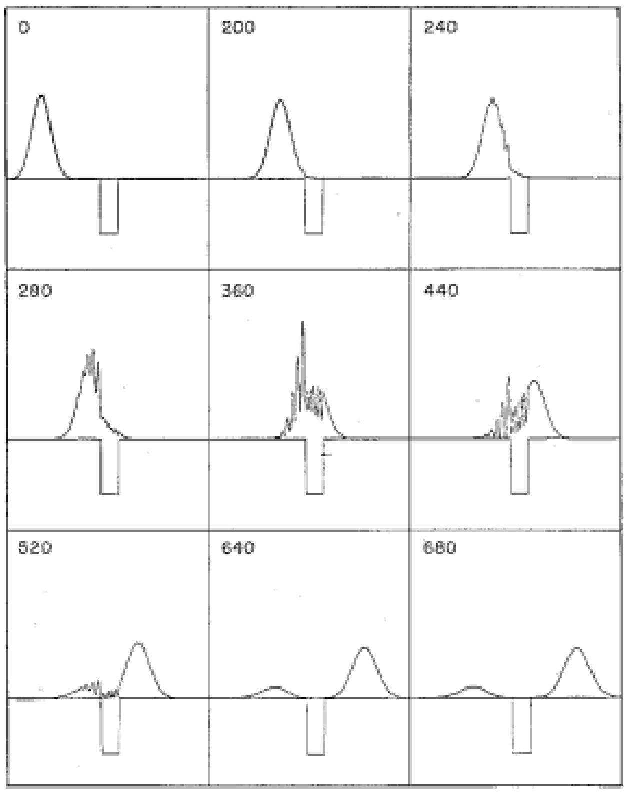

FIG. 1. Gaussian wave-packet scattering from a square well. The average energy is one-half the well depth. Numbers denote the time of each configuration in arbitrary units.

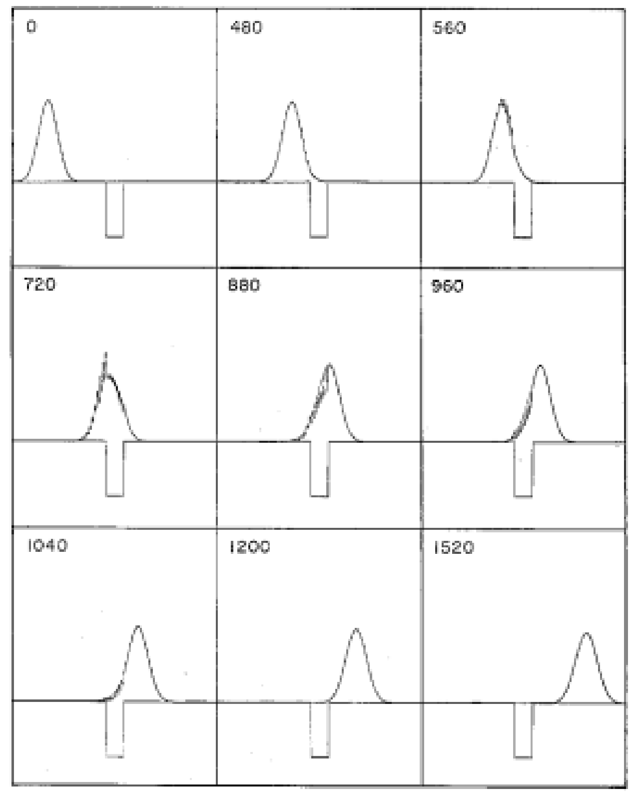

FIG. 3. Gaussian wave-packet scattering from a square well. The average energy is twice the well depth. Numbers denote the time of each configuration in arbitrary units.

A. Goldberg, H.M. Schey, and J.L. Schwartz, Am. J. Phys. **35**, 177 (1967)

simple way to avoid this problem; but, fortunately, the discontinuities, while annoying, by no means destroy the effect of the film. 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. Our feeling, nonetheless, is that despite their shortcomings these films already have considerable merit as a pedagogical tool and, as methods are refined and scope broadened, they will play an increasingly important role in science teaching both at the college and graduate levels.

ACKNOWLEDGMENTS

The authors are deeply grateful to Raymond L. Tarp, who expertly programmed all computations and plotting routines involved in this project. We wish also to thank Dr. Cecil E. Leith for an important conversation. Computations for this work were done on the Livermore IBM-7094 and CDC-3600.


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"That's all Folks!"