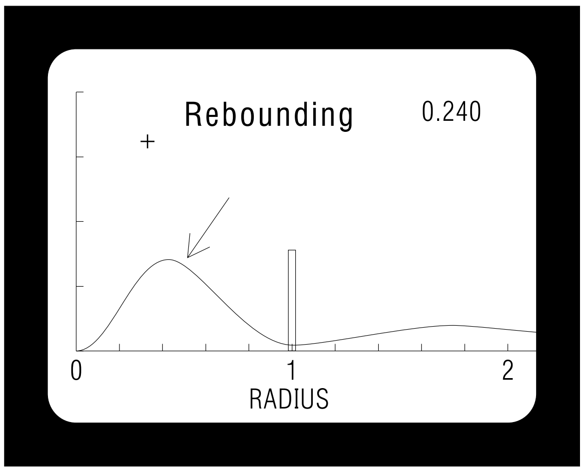
PHYSNET

MISN-0-265

QUANTUM TUNNELLING



Project PHYSNET Physics Bldg. Michigan State University East Lansing, MI

QUANTUM TUNNELLING

by

Peter Signell

Title: **Quantum Tunnelling**

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Input Skills:

1. Vocabulary: de Broglie waves, quantum probability density (MISN-0-240); turning points (MISN-0-22); exponential probability decay law (MISN-0-264).
2. Given a one dimensional potential energy curve and a particle's total energy, describe the particle's motion. Include trapped particles and untrapped particles (MISN-0-22).
3. Outline the graphical method of determining whether or not a given set of data is consistent with an exponential description. Sketch illustrative examples (MISN-0-264).

Output Skills (Knowledge):

K1. Correlate a tunnelling wave packet's evolving behavior with general properties of the Schrödinger equation and with periods of exponential and non-exponential decay.

K2. Show that quantum tunnelling violates expectations from classical mechanics.

K3. Discuss your reaction to the probabilistic basis of quantum mechanics.

External Resources (Optional):

1. *Quantum Tunnelling in Radioactive Decay*, a motion picture, Project Physnet, 1993. For access, see this module's *Local Guide*.

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1. "Seeing" Quantum Tunnelling

1a. Quantum Tunnelling. One of the most startling predictions of quantum mechanics is that the wave nature of particles enables them to tunnel through classically-impenetrable barriers. This mechanism constitutes the traditional model of α-particle decays found in natural and induced radioactivity, wherein an alpha particle which had been classically trapped inside a nucleus is found to have escaped through the surface barrier. It also governs the tunnelling of electrons through classically-impenetrable surfaces and layers, an effect that is important in many electrical and electronic devices.

1b. Equation Generation of Pictures. The physics equation which allows and governs quantum tunnelling can be made to show us the details of the process. This is accomplished by solving the equation on a computer for a particular system at various times. The resulting solutions at the times of interest can be plotted as graphs with any scales one wishes along the graphs' axes. The graphs can even be combined to make a motion picture, a movie, of the tunnelling. For example, an equation-generated movie of an α-decay can be made to take several minutes and be the size of a movie screen, although the decay actually takes place in a region about 10^{-12} cm in diameter and in about 10^{-18} sec. This means we can observe the process at leisure and "see" how quantum mechanics allows an object to get through an "impenetrable" barrier. As a byproduct we will also be able to see how quantum mechanics interprets the "no-aging" assumption of the traditional Exponential Decay Law for escape through such a barrier.

1c. Quantum Probability Density and Probability. Quantum mechanics (QM) specifies the relative probabilities of finding an object at various places at various times. Thus we can solve the relevant QM equation to find an object's radial probability density, P, at radii and times of interest. Then we can calculate the total probability P of finding the object somewhere in a region by determining the area under the density curve in that region. For example, the total probability of finding the object somewhere in the region bounded by the radii r_1 and r_2 at time t

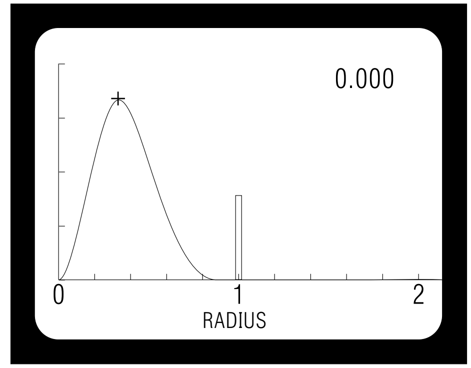

Figure 1. Probability density $p(r,t)$ versus radius at time 0 for a nuclear α-particle. The vertical bar at unit radius represents a spherical nuclear surface-barrier potential.

is just the area under the probability density curve between r_1 and r_2 at that time (see Appendix A).

2. Evolution of a Trapped Wave Packet

2a. Probability Density at $t = 0$. Picture a nucleus as a hollow sphere of unit radius inside of which we place a wave packet representing an α-particle. This is illustrated in Fig. 1, where a time-zero radial probability density p is plotted versus radius.[1] The vertical bar at unit radius indicates there is a spherical barrier at that radius, of the thickness shown. This barrier is due to a "surface tension" at the nuclear surface. Classically, this barrier keeps particles inside the nucleus since they would have insufficient energy to penetrate it.[2] The quantum probability $P(t)$ of finding the α-particle "inside the nucleus" at any time t is just the appropriate area under the probability density curve at that time: $P(t)$ = area under $p(r,t)$ between $r = 0$ and $r = 1$. This is the probability that the nucleus has not decayed by time t, since it is the probability that the α-particle is still somewhere inside. The curve shown in Fig. 1 is for time zero, the instant of creation of the radioactive nucleus. Thus 100% of the probability is inside the surface at that time:

$$P(0) = \text{ area under the curve at time zero } = 1.00$$

[1]The shape of the wave packet shown in Fig. 1 was chosen as a plausible one which might result from a real creation process. The "inside" wave function is the product of a sine function and an exponential function, while the "outside" one is zero. Schrödinger's equation demands that the probability density be zero at the origin: [see "The Schrödinger Equation in One Dimension: Quantization of Energy" (MISN-0-242)].

[2]See "Potential Energy Functions and Motion" (MISN-0-22).

2b. Probability Density Evolution ($t \geq 0$). If we now let time start rolling in Fig. 1, we get the time sequence shown in Fig. 2. The time dependence shown here was generated by solving the time-dependent Schrödinger equation[3] on a computer.

Scan the columns of Fig. 2 from top to bottom consecutively, creating a sort of movie impression of the motion in your mind's eye. Notice that the wave packet, representing the α-particle, hits the barrier and rebounds from it several times before settling down to a steady fading shape. Times are shown in the upper right corner of each frame. The plus sign (+) in the upper left part of each frame is the position of the probability peak at time zero.

The motion between time zero and the first time the packet hits the barrier is shown in detail in the first column of Fig. 3; the motion during the first rebound is detailed in the second column. By scanning down the columns of Fig. 3 you should be able to get a feeling for the motion during those time intervals. Notice, in particular, the pulse of probability which moves through the barrier and escapes following the first impact (right column, Fig. 3).

2c. Probability Evolution ($t \geq 0$). We can find the area under the curves inside the barrier for each of the frames shown in Figs. 2 and 3, as well as in frames between those shown,[4] but are the same as those shown in Figs. 1, 2, 3. Note the straight-line exponential region. Thus we can accumulate a sequence of $P(t)$ values showing the time development of the probability left inside the surface. In order to determine whether this probability is exponentially decaying, we can plot the logarithm of $P(t)$ versus time.[5] For the system we have just seen in Figs. 1-3, the graphs of $\ell n\, P(t)$ and $\ell n\, [\text{decay-rate}(t)]$ are shown in Figs. 4 and 5. Notice that the decay becomes rather exponential after $t \simeq 0.6$. Looking back at Fig. 2, one sees that this is the time region where the probability density settles down to a constant radial shape and then just fades away. A wave intensity which maintains a space-constant shape like this is usually called a standing wave.[6]

[3] See "The Time-Dependent Schrödinger Equation: Derivation of Newton's Second Law" (MISN-0-248).

[4] See Appendix A, "The 'Counting Squares' Technique for Numerical Integration" for method and Appendix B, "Wave Packet Graphs During Exponential Decay" for blow-ups of individual stills.

[5] See "Exponential Decay" (MISN-0-264).

[6] See "Standing Waves" (MISN-0-433) for an elaboration and "Resonance Modes in Membranes" (MISN-0-233) for interesting examples.

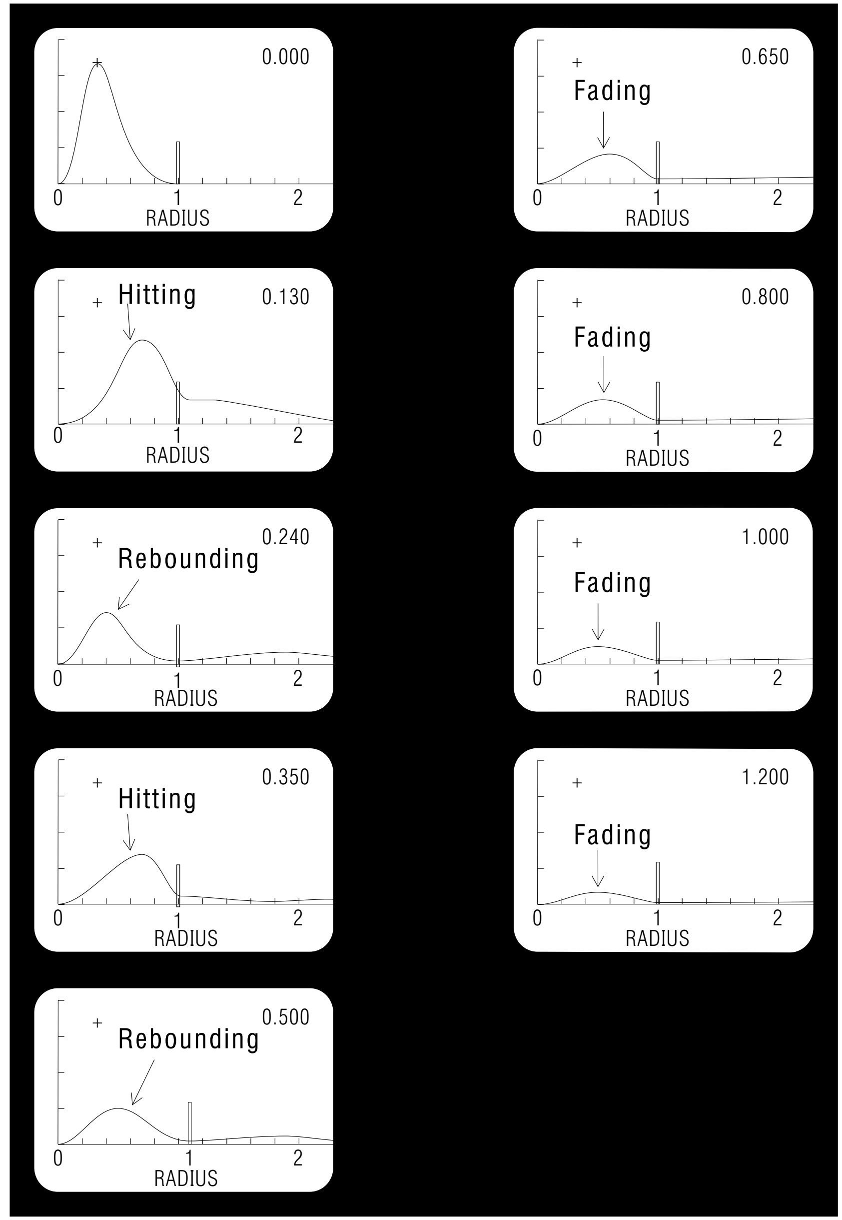

Figure 2. Probability leaking through a barrier. Times are shown in the upper right corner of each frame.

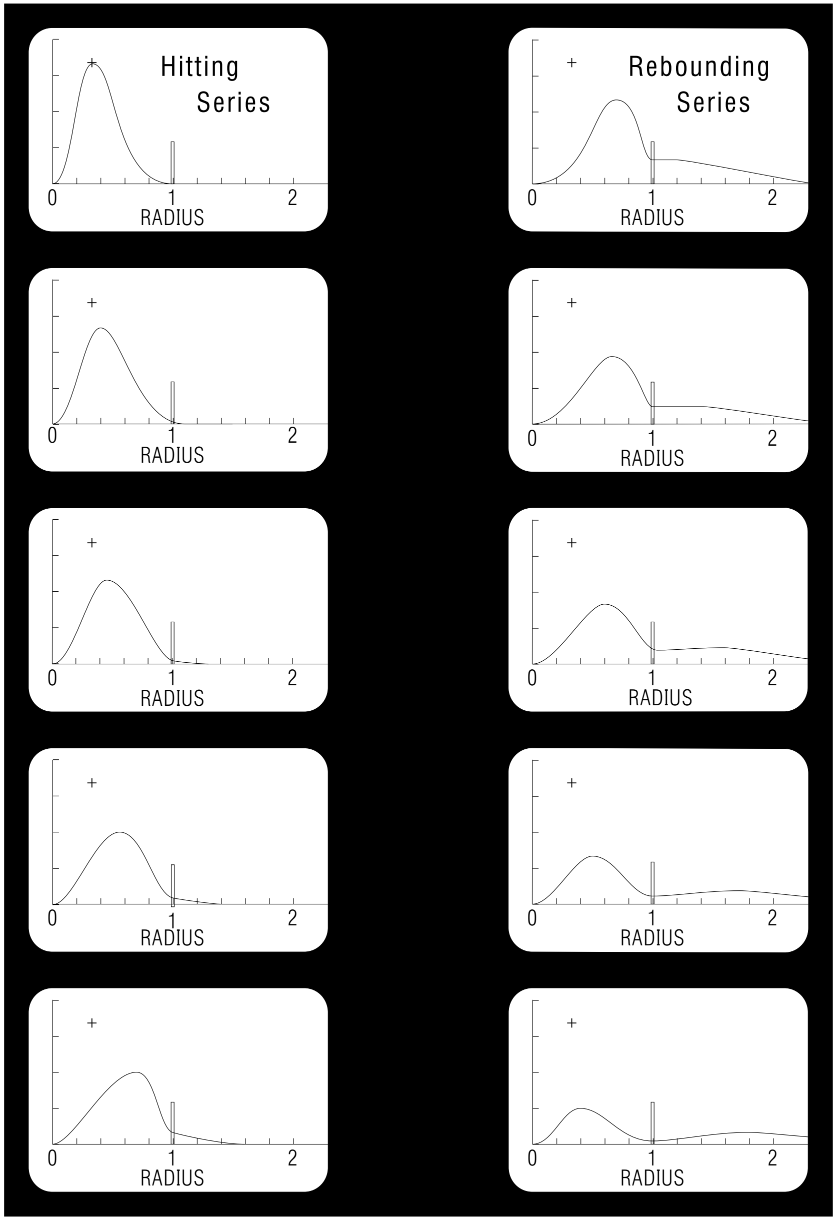

Figure 3. Frames between the first three of Fig. 2.

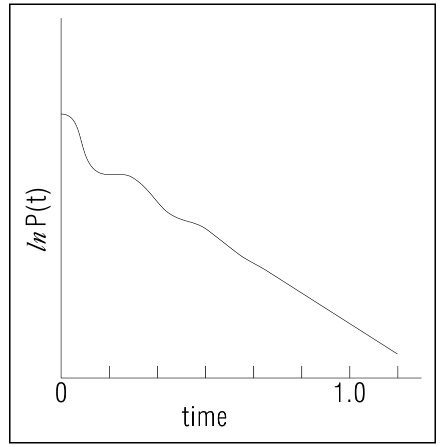

Figure 4. Plot of $\ell n\, P(t)$ vs t. The time units are unspecified but are the same as those shown in Figs. 1, 2, 3. Note the straight-line exponential region.

We conclude that a particle-like motion throughout the interior, with reflections from the walls, allows pulses of probability to escape and produces non-exponential decay. A standing wave allows the probability to steadily seep out and produces exponential decay.

2d. Interpreting "No-Aging" Exponential Decay. The standing wave aspect of exponential decay gives an interesting interpretation to the traditional "no-aging" assumption of the widely-used exponential decay law. This assumption is that the character of a decaying system does not change with time, that the system does not "age" until the instant of decay. The no-aging assumption manifests itself, in the usual derivation

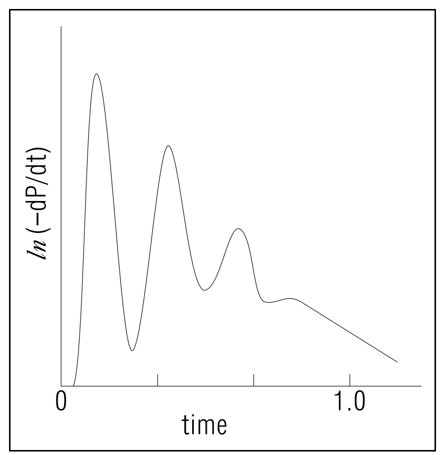

Figure 5. Plot of the log of the rate at which probability escapes through the barrier. Note the straight-line exponential region.

of the exponential decay law,[7] through the use of a time-*independent* "decay constant." We can now interpret this "constant decay-constant" or "no-aging" assumption as saying that, for exponential decay times, the system must be a standing wave so the *shape* of its probability distribution is constant as time changes. Then we see no change in the system's character during exponential decay times, only a steady decline in the system's probability of not having decayed. [Q1-6][8]

2e. Three Segments in a Lifetime. Pure exponential ("non-aging") decay is only a mathematical approximation to a particular segment in the lives of real decaying systems. In reality, decaying systems continuously "age." An early non-exponential decay rate is often followed by a long period when the rate is very close to being exponential. Quantum mechanics says that this period is followed, in turn, by a period when the decay rate approaches a time-to-a-negative-integer-power (t^{-n}) behavior. The transition between the latter two periods can show oscillating probabilities, including some times when the decay rate is negative.[9] We can summarize by saying that a decaying system's youth is often spent in knocking about, with middle age being characterized by an imperceptibly slow change of character. This is followed by a transition period of strange oscillations and then an old age with a "decay constant" which decreases with time.

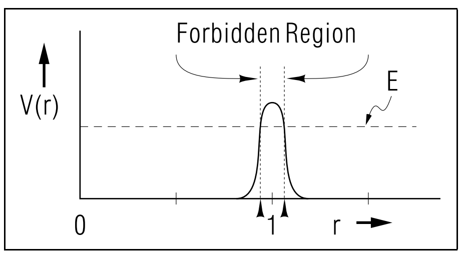

Figure 6. The same spherical-shell potential as in Figs. 1-3, but with rounded edges. A trapped particle's energy is indicated by E, its turning points by arrowheads.

3. Classical Expectations, Tunnelling

3a. Classical Trapping by a Potential Barrier. What does classical mechanics predict for the motion of the particle created inside a spherical-shell barrier at time zero? In order to make the answer easier to obtain, we replace the previous potential with one rounded at the edges as in Fig. 6. For any particular particle energy, such as that shown in the figure, there are two turning points; one for a particle classically trapped inside the barrier and one for a particle which, classically, is forever outside the barrier.

All that prevents an inside particle from escaping is the classically forbidden region between the two turning points, where its kinetic energy would have to be negative and hence its velocity imaginary. If an inside particle could penetrate this forbidden region and somehow tunnel through it to the outside turning point, it would then be accelerated away from the surface and would escape. We would detect it, far from the surface, with a kinetic energy just equal to the total energy it had while inside the surface: we would say that the system had decayed by emission of a particle. Classical mechanics can neither describe nor explain the "tunnelling" part of that process.

3b. Schrödinger Equation Tunnelling. How does quantum mechanics allow a particle to tunnel through a barrier? The equation governing the behavior of deBroglie-Schrödinger waves, called the Schrödinger equation, has some of the characteristics of both wave equations and diffusion equations.[10] The hitting and rebounding of the probability from the barrier shows a wave characteristic similar to, say, a water wave being reflected from a sea wall. The quick broadening of the peak to a much more even distribution, followed by a gradual seeping through the barrier, shows a diffusive characteristic similar to, say, the diffusion of concentrated sugar water to a region of lower concentration on the other side of a semi-permeable membrane. There, also, initial irregularities quickly dissolve into a more even, steadily decreasing concentration.

[7] This 3-line derivation uses simple calculus; see "Exponential Decay: Observation, Derivation" (MISN-0-311).

[8] Q1 refers to Question 1 in this module's Special Assistance Supplement.

[9] See "Evolution of a Quasi-Stationary State," R.G. Winter, Phys. Rev. *123*, 1503 (1961) and "Large-Time Exponential Decay and 'Hidden Variables'," R.G. Winter, Phys. Rev. *126*, 1152 (1962).

[10] For an examination of the diffusion equation some typical solutions, see "The Diffusion Equation: Derivation and Solution" (MISN-0-171).

3c. Probability in the Forbidden Region. One can easily calculate the appropriate areas to find the amounts of probability between the turning points in Figs. 2 and 3 and hence find the numerical probability that the particle will be in a region of imaginary velocity! Does quantum mechanics really say that the mean velocity of the particle is imaginary there? More or less "yes,"[11] but it also says that the particle could only be observed to be in that region if the observer supplies enough energy to it to allow the particle to have a real velocity. Such an observer would then deduce that the particle's kinetic energy had been negative by comparing the supplied energy with the observed kinetic energy. Thus the detected velocity is real, although the undisturbed velocity in that region can be said to be imaginary. [Q7-10]

4. Reactions to Qm Probability

4a. Probabilistic Nature of Quantum Information. The great Schrödinger equation, which apparently contains all of the secrets of chemistry and biology, says nothing whatever about how our particle got through the barrier and escaped. Yet it states precisely how the particle's probability got through the barrier. One is left with the impression that the question of how the particle itself got through the barrier is not even a meaningful question in the atomic domain.

4b. Attempts to Escape QM Probability. The idea of a probabilistic reality is so unacceptable to some physicists that they assign the probability density a material aspect in their minds, thinking of it as the goo of which the particle is made. It is obvious that such a picture is misleading: when the half-life time arrives, for example, one does not find half the particle (or half its goo) outside the barrier. Rather, if one repeats the experiment many times ($N \Rightarrow \infty$), one finds that in 50% of those trials the whole particle had escaped while in the other 50% of the trials the whole particle was still inside at the half-life time. The probabilistic picture seems inescapable.[12] The discovery of this probabilistic character of quantum phenomena so disturbed Albert Einstein that he bowed out of further participation in the development of quantum physics and spent most of the last 25 years of his life working in other areas.

[11] Velocity is not really defined in quantum mechanics but, as here, can be assumed to be momentum divided by mass, a quantum mechanical quantity.

[12] The Everett-Wheeler Hypothesis is a bizarre picture that makes quantum mechanics seem completely causal and mechanistic. This hypothesis neither adds to nor changes the usual quantum mechanical predictions, so most physicists do not show much interest in it. The small fraction of physicists who worry about quantum measurement theory seem to have stronger pro and con opinions regarding the Everett-Wheeler hypothesis. Another avenue of approach is discussed in "Hidden Variable Theories" (MISN-0-269, UC), although recent evidence is strongly against hidden variable theories.

4c. Interpretation of the Desire to Escape Probability. Why do some of us find a probabilistic interpretation so unfulfilling, rather than being thrilled by the difference from appearances on the every-day macroscopic level? One hypothesis is that when certain individuals learn of such a departure from their total past experience and belief, they find it unusually difficult to accept the new concept.[13] Another hypothesis is that perhaps such persons go into physics with the expectation that it will enable them to work with certainties, as opposed to the uncertainties of personal interactions. They believe that the universe should basically work like a watch with intermeshed gears all exactly driving each other.

It is not always fruitful to downgrade such beliefs. Physics often seems to advance because someone tenaciously investigates a line of research resulting from an intuitively—or emotionally-based belief. Such essentially religious motivations are a recurring element in the progress of science. This does not necessarily mean that they are beneficial on the average, however, since they can also constitute a brake on creativity.

4d. Projected Reaction to an Underlying Mechanism. If, some day, someone shows that there is a deeper level than quantum mechanics, a level in which nature is again mechanistic, and if this discovery results in startling new insights and fields of development, that person will become an instant celebrity in the physics world. For fifty years, however, the probabilistic aspect of quantum mechanics has completely withstood all assaults. Now what is your personal reaction to the probabilistic nature of quantum mechanics? [Q11]

Acknowledgments

Professor Rolf Winter first interested the author in this area and devised the basic model. Jonas T. Holdeman, Jr. discovered a key part of the algorithm used in solving the time-dependent Schrödinger equation on the computer. Tom Burt, Julie Junttila, and Chuck Taylor participated in the film production, for which Paul Timnick was the staff artist. Tom Burt

[13] It is easy to demonstrate that incoming optical and acoustical information is often altered by your brain in order that you will perceive a false concordance with previous experience.

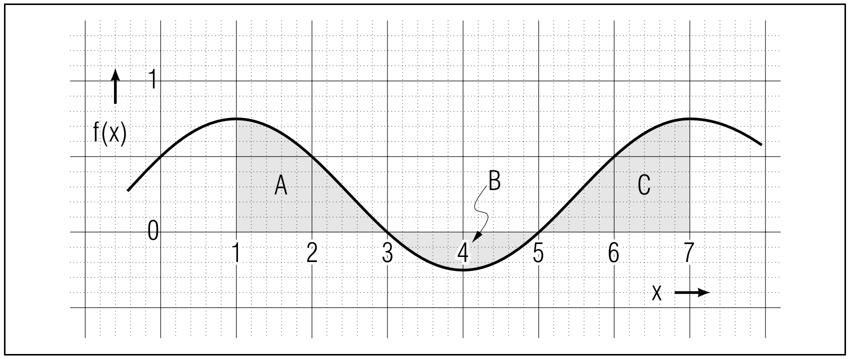

Figure 7. The integrals in each of the three regions shown are: $A = 0.91$, $B = -0.32$, $C = 0.91$.

and Jonas Holdeman also coordinated much of the effort. Preparation of this module was supported in part by the National Science Foundation, Division of Science Education Development and Research, through Grant #SED 74-20088 to Michigan State University.

A. Area by "Counting Squares"

Suppose one needs the area under a function which is only defined by a series of points. Without knowledge of the functional form of the curve, one must resort to some form of numerical integration or area measurement. An appropriate method for the present case is that of "counting squares." As an example of the method, consider the curve of Fig. 7, for which the desired area is between the limits $x = 1$, and $x = 7$. The regions A and C must be evaluated separately from B, where the values of the curve are negative. To evaluate the area under, say, region A, pick as basic squares either the small squares or the large darker-line ones which enclose 25 smaller squares. Then count the number of your basic squares that are enclosed by the boundaries of region A. If the curve cuts through a square, estimate what fraction of the square is under the curve. Normally, such estimates have surprisingly good accuracy. Using the large squares as basic, you should find that region A contains 1.82 ± 0.02 of them. That's an accuracy of 1%! Now obtain the scale factor between your squares and the $f(x)$ scale by either finding the amount of graph area for a given number of squares or by finding the number of squares between definite x- and y-coordinate intervals. For example, since there are two large squares between the intervals $(0 < x < 1;\ 0 < y < 1)$, there

are two such squares per unit function area. This means that the true area of the region A is 0.91. Similarly, you should be able to find the areas of B and C given in the caption to Fig. 7. The total area is then:

$$\text{Area under } f(x), 1 \leq x \leq 7 = 1.50$$

B. Wave-Packet Graphs

Figure 8 shows a sequence of wave packet probability distributions during exponential decay, suitably enlarged for numerical integration. The inverse of the decay constant, the mean life, can be shown to be close to 0.68 for this case.

C. A Motion Picture

The three minute movie "Quantum Mechanical Tunnelling Through a Barrier" is available. For access, see this module's *Local Guide*. This film was produced by animation of computer solutions.[14] to the time-dependent Schrödinger equation for the case shown in Fig. 1.

[14] See "Unitary Pade Algorithm for Solving the Time-Dependent Schrödinger Equation" (MISN-0-312), wherein the relevant computer algorithm is derived (under construction).

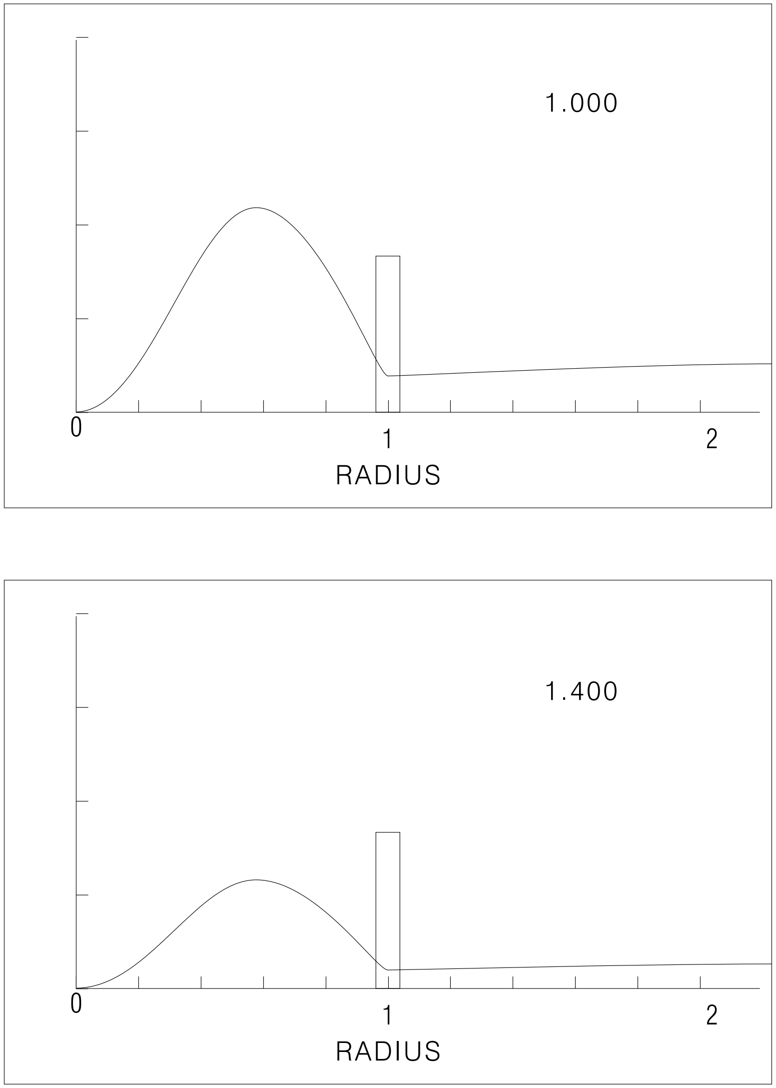

Figure 8. As in Fig. 2 at several times, enlarged.

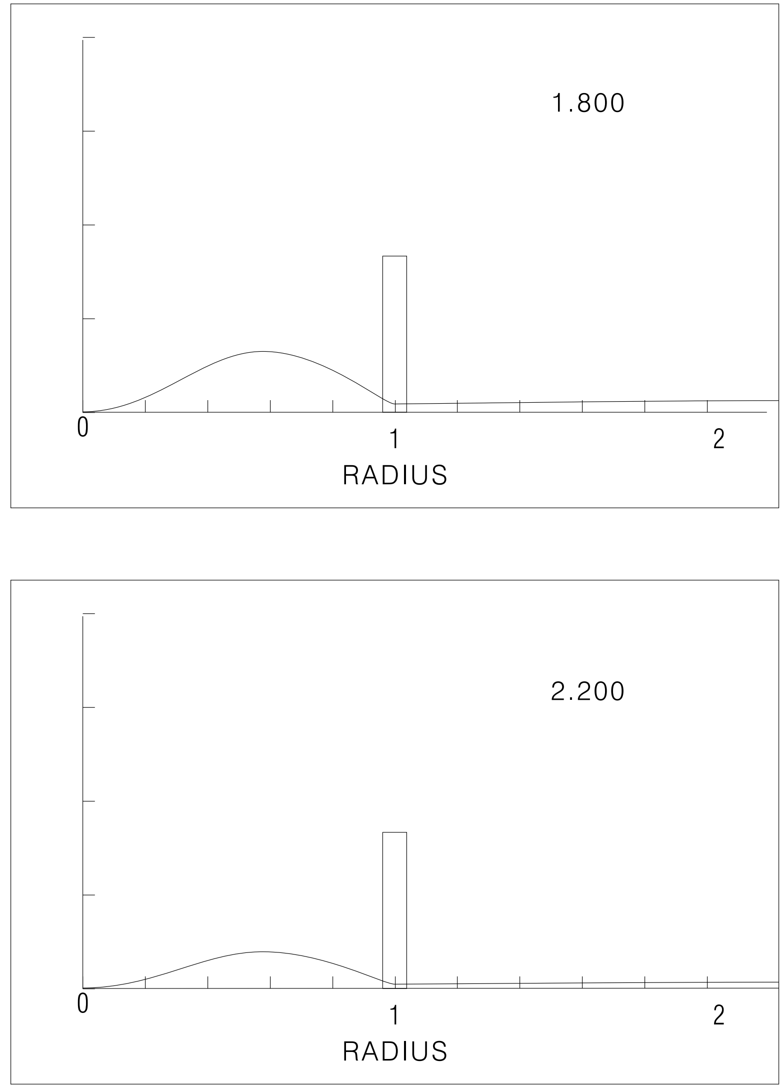

Figure 9. Continuation of Fig. 8.

LOCAL GUIDE

The three-minute movie is available in the course's Consulting Room. If you want to see it, go there and ask the Consultant to get the personal projector and movie cartridge out of the bottom drawer of the cabinet and to set it up for you. Be aware that the projector's light beam must be aimed at the mirror at the proper angle so as to fully illuminate the personal screen from the rear.

SPECIAL ASSISTANCE SUPPLEMENT

Q1. Describe the motion of a trapped wave packet during the early and later stages of decay.

Q2. Why is the probability inside the barrier equal to 100% at $t = 0$?

Q3. The probability density distribution shown in Fig. 1 looks considerably higher than the barrier. Is this significant or is there no relationship between the two heights on the graph?

Q4. Can you visualize the hittings and reboundings shown in Fig. 3, and identify them in Fig. 2?

Q5. Why do the shapes of the curves in Figs. 2, 4, and 5 demonstrate that particle-like motion produces non-exponential decay, while standing waves correspond to exponential decay?

Q6. What is the connection between the detailed shapes of Figs. 4 and 5 during the first wiggle and the time of the first hitting, rebounding, and escaping pulse of Fig. 3?

Q7. Can you relate characteristics of the Schrödinger equation to the two regions of Figs. 4 and 5?

Q8. How can one reconcile the statement that the Schrödinger equation predicts imaginary velocities with the fact that observed velocities are real?

Q9. Consider a particle heading outward from the origin, heading toward the barrier in Fig. 6. What is the particle's classically-predicted velocity as a qualitative function of both radius and time?

Q10. Can you show algebraically that velocity would be imaginary if a particle's potential energy exceeded its total energy?

Q11. What is your personal reaction to the probabilistic basis of quantum mechanics? Do you accept it or reject it? On what grounds?

Brief Answers:

The answers to the questions posed above are either in this module's *text* or are meant to be personal answers.

MODEL EXAM

1. See Output Skills K1-K3 in this module's *ID Sheet*. The actual exam will include one or more of these skills.

Brief Answers:

1. See this module's *text* and think and argue with your colleagues.