Qualitative Plots of Bound State Wave Functions

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Qualitative Plots of Bound State Wave Functions

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When students are introduced to the one-dimensional Schrödinger equation, there is a tendency to limit its application to a few forms of potential for which exact analytic solutions are readily obtainable—notably, of course, the simple square well. We have found, however, that students can easily be trained to make qualitatively correct pencil and paper plots of stationary state wave functions for arbitrary one-dimensional binding potentials. This developed ability gives the student a chance to take a first rough cut at a new problem, gain a qualitative insight into the properties of a particular state, and achieve an independent basis of judgment as to whether or not an analytic formula or a computer-generated solution is approximately correct. Moreover, the same skill can be used in analyzing three-dimensional systems that are analytically separable into equivalent one-dimensional problems. We suspect that many instructors have discovered the usefulness of qualitative plots in teaching quantum physics, but to our knowledge the results have not found their way into textbooks.

The essential background for making qualitative plots is a knowledge of the de Broglie relation, a (largely implicit) understanding of the continuity requirements on the wave function, and an acquaintance with the exponential-type decrease of the wave function with distance into any classically forbidden regions. In addition to this minimum background, our students have had a first contact with the time-independent Schrödinger equation and have solved the finite square well problem using graphical methods.

An emphasis on the importance of curvature begins the conversion of square-well results to the more general case of potentials that vary with position. The lowest possible energy state, for example, implies the smallest possible momentum at every point in the potential, which implies the longest possible "local wavelength," which implies the smallest possible curvature of the wave function consistent with matching to the decaying functions at the boundaries. The second energy state

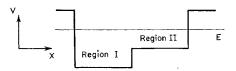


Fig. 1. Potential plot used to analyze peak heights of wave function as a function of well depth.

wave function has the next-higher local curvature at every point consistent with the boundary conditions. These results are applicable also to space-varying potentials and lead to the following common features of every stationary state wave function in a onedimensional potential.

- 1. The wave function for the nth energy level has n-1 nodes.
- 2. Inside the well the "local wavelength" is longer in shallower portions of the potential well.
- 3. Inside the well the amplitude of the wave function (the height of the peaks) is greater at places where the well is shallower. (This point is discussed more fully below.)
- 4. Wherever the potential energy V is greater than the total energy E, the local "exponential decay constant" of the wave function with distance is greater for a larger value of V-E.
- 5. In potentials that are symmetrical with respect to a given point, stationary state wave functions are alternately odd and even with respect to the point of symmetry, the lowest-energy wave function being even.

Statement 3 may not be generally appreciated, even among professionals. That it follows directly from the de Broglie relation plus continuity requirements can be seen from a simple example. Consider a solution of energy E in the step potential shown in Fig. 1. Within the well the solutions are sinusoidal:

$$\psi = A \sin(kx + \phi)$$
 (inside well), (1)

where $k=2\pi/\lambda=p/\hbar$. The values of A, k, and ϕ will, in general, each be different for regions I and II. We want to show that the maximum value A is larger in region II than in region I. This is done by considering the slope $d\psi/dx$ of the wave function. Call this slope m. Then

$$d\psi/dx = m = Ak \cos(kx + \phi)$$
 (inside well). (2)

Rewrite (1) and (2) as

$$\sin(kx+\phi) = \psi/A$$
,
 $\cos(kx+\phi) = m/kA$.

These equations can be squared and added to eliminate the phase ϕ and yield an expression for the maximum value A:

$$A = (\psi^2 + m^2/k^2)^{1/2}$$
 (inside well). (3)

Now recall that both the value of ψ and its slope m are continuous across the step, but that the value of k changes discontinuously. Continuity demands that infinitesimally close to the step the values of both ψ^2 and m^2 in Eq. (3) have the same magnitude on either side. Therefore at the step the maximum value A of the wave function *increases* as k decreases (except for the special case m=0). The momentum p (and hence the

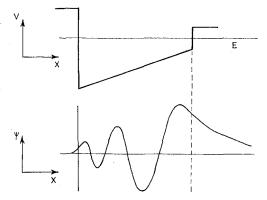


Fig. 2. Sample qualitative plot of wave function for the fifth energy level in a ramp-bottomed potential well.

wave number k) is smaller in region II than in region I. Therefore the maximum value A is greater in region II than in region I. QED

In the special case that the slope m equals zero at the step, continuity can be maintained with the same value of A in both regions.

Now, any potential function whatever can be approximated by a series of superposed step functions. The preceding analysis is valid for each such step, so

the conclusion can be applied to any continuously varying potential, and thus to a potential well of any shape: regions of smaller momentum have larger maximum values of the wave function than regions of larger momentum. This completes the analysis of feature number 3 in the list above.

We have found that students are able to draw a wave function without error in any of the five features listed above provided they are given the drawn figure of the one-dimensional potential, are told which energy level it is (for example, the fifth), and have the energy of the level indicated by a horizontal line drawn on the potential plot. Figure 2 shows just such a case. One reason that qualitative plotting works so well from a pedagogic point of view is that, by indicating the energy on the potential plot and giving the state number, we provide implicit dimensional scales of distance and energy that allow the student to ignore, for the limited purposes of a rough plot, the magnitudes of Planck's constant and the mass of the trapped particle that lie behind atomic units of distance and energy.

Single copies of programmed study material, introducing qualitative plots of this kind, are available without charge through the Education Research Center, Room 20C-228, Massachusetts Institute of Technology, Cambridge, Mass. 02139.

A Student Experiment on Successive Radioactive Decay

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An experiment which would demonstrate the principles of successive radioactive decay was required as part of an undergraduate laboratory course in reactor and nuclear physics, the intention being to measure the decay constants of the chain members. There were a number of restrictions on the choice of chain to be investigated. A chain with two active members presents a sufficiently complex problem and makes it feasible that the experiment be performed and the calculations completed in the course of one 3-h laboratory period, provided that the half-lives in question are of the order of minutes. The parent isotope had to be produced in a measurable quantity by neutron irradiation in a research reactor (in a thermal neutron flux of approximately 10¹² cm⁻² sec⁻¹) for a time short compared with either the parent or the daughter half-life, that is for a few seconds. Both parent and daughter substances should emit γ radiation so that the decays can be easily followed using scintillation detectors which should also allow the decays to be distinguished one from the other. Finally, there should be negligible contamination by other active isotopes.

Examination of the decay schemes of the active isotopes accessible by neutron activation showed that the only chain meeting the above (fairly exacting) requirements was:

The values of the half-lives are those given by Lederer et al.¹ It should be mentioned that, while the value 14.6 min for the ¹⁰¹Mo half-life has been obtained by three different investigators, there is a spread in the values quoted for the ¹⁰¹Tc half-life, the value 14.0 min having been found most often.

About 100 mg of molybdenum oxide (MoO₃) irradiated for 5 sec in the above thermal neutron flux yields sufficient activity to be measured with good statistical accuracy in a counting time of 30 sec. A series of such counts at 1-min intervals over a period of an hour or so gives enough data to show the decay of