



RECTANGULAR POTENTIALS

Quantum
Physics

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

RECTANGULAR POTENTIALS

by
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Input Skills:

1. Solve two simultaneous algebraic equations with two unknowns.
2. Unknown: assume (MISN-0-384).

Output Skills (Knowledge):

- K1. Write down the solution to the S-equation in a region of constant potential V , for the case $E > V$ and $E < V$.
- K2. Write down the boundary conditions applying to the wave function at a point of discontinuity in the potential.

Output Skills (Rule Application):

- R1. Use the boundary conditions of K2 to relate the amplitude coefficients of the wave functions in the various regions. In the case of scattering states ($E > V$ in the region from whence the wave packet is incident), the direction of motion of the incident packet must be taken into account.
- R2. Apply the definition of the probability current to calculate reflection and transmission coefficients in the various regions.

Output Skills (Problem Solving):

- S1. Determine the energy eigenstates and energy eigenvalues for the infinite square well in one dimension.
- S2. Solve problem 5.13. In addition, the student must be able to calculate the expectation values of all the operators in table 4-2 in infinite square well eigenstates.

External Resources (Required):

1. E. E. Anderson, *Modern Physics and Quantum Mechanics*, W. B. Saunders (1971).

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New authors, reviewers and field testers are welcome.

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1. Introduction

In this unit we shall attack our first class of problems to be solved with the Schrödinger equation. In these problems the potential has sharp discontinuities, but is constant in the regions between the discontinuities. While such potentials are not physically realistic, our study will reveal some general characteristics of solutions to the energy eigenstate problem. Furthermore, when the potential is unknown (as is frequently the case in research) rectangular potential solutions are frequently used as “zeroth-order” approximations to the wave function in order to get a theoretical starting point.

2. Procedures

The material for the unit is covered in sections 5.1 to 5.3 of Anderson. In each section a slightly different potential is discussed but the basic method is the same; and learning this method constitutes the first three Output Skills.

1. Read section 5.1, skipping the reflection and transmission coefficients for the time being. Be sure you understand equations (5.1), (5.2), and (5.8); the steps leading to them, and how and why they differ. You must be able to derive these equations from memory. A , B , C and D are the “amplitude coefficients.” Why must D be zero in each of the two cases?
2. The boundary conditions (5.4) must hold at *any point* (there is nothing special about $x = 0$) for any physical wave-function ψ . These plausible conditions require that physical states be represented by probability distributions with no discontinuities or “sharp points.”
3. Imposing the boundary conditions (5.4) on equations (5.1) and (5.2) leads to equations (5.5). In a similar way (5.9) is obtained. Make sure you can derive these relations among the amplitude coefficients.

► In the center of page 161 Anderson meant to write:

$$k_2 = \imath K_2 .$$

4. Let us return now to the transmission and reflection coefficients. In Chapter 4, we skipped section (4.10) in which the *probability current* \vec{S} was defined by:

$$\vec{S} = \frac{\imath\hbar}{2m} \left[\Psi(\vec{\nabla}\Psi^*) - \Psi^*(\vec{\nabla}\Psi) \right] .$$

Here \vec{S} is analogous to the Poynting Vector in electricity and magnetism and represents the probability flow per unit area per unit time. Conservation of total probability in time is expressed by:

$$\vec{\nabla} \cdot \vec{S} + \frac{\partial \rho}{\partial t} = 0 ,$$

where ρ is the probability density. What can you say about \vec{S} in a region where Ψ is real, or where the phase of Ψ is independent of position?

Note that \vec{S} depends on time through Ψ . However, for stationary state of energy E ,

$$\Psi(\vec{r}, t) = \psi_E(\vec{r})e^{-\imath Et/\hbar} .$$

Show that, for such a state, \vec{S} is independent of time and given by the same expression but with $\Psi(\vec{r}, t)$ replaced by $\psi_E(\vec{r})$.

The transmission and reflection coefficients are, by definition:

$$T \equiv |\vec{S}_{tr}|/|\vec{S}_{in}|, \quad R \equiv |\vec{S}_{re}|/|\vec{S}_{in}|$$

where the subscripts denote the transmitted, reflected, and incident waves. Armed with this knowledge, derive equations (5.7) and (5.10). The coefficients are the percentage of the incident probability transmitted and reflected—for one particle incident they represent the probability of finding the particle on either side of the barrier after the collision.

Note that we are using the language of a time-dependent collision process, even though we are working with time-independent energy eigenstates. This is done for convenience—it would be better (certainly more intuitive) to give a time-dependent treatment with physical *wave packets*; but this is too complicated for us to take up here.

The price we pay is having to make some plausible, but not completely justified, identifications of various *parts* of the wave function with different time-dependent phenomena (reflected wave, transmitted wave, etc.). The more correct time-dependent approach would vindicate our assumptions.

(1')-(4') Now go on to section 5.2, paying attention to the same points as in (1)-(4) above. Only the shape of the potential has changed. Note that for certain energies, there is 100% transmission through the barrier; an interesting and purely quantum mechanical effect. To gain practice in obtaining practical results, solve problems 5-3, 5-4, 5-5 and 5-6.

► On page 166 Anderson seems to imply that 10^9 seconds is equal to 100 years; actually it is equal to about 30 years.

5. Read section 5.3. Here we have a *well* instead of a *barrier* and for energies less than the height of the well, *bound states* are obtained, i. e. ψ goes to 0 at $\pm\infty$, indicating that the particle is bound to the potential (states like these correspond to electrons bound in atoms).

Study the derivation of the conditions on the amplitude coefficients. Be sure you see why the wave function must be even or odd.

In the case of the infinite well, the wave function must vanish outside the well to avoid having infinite energy. (In this idealized case, $d\psi/dx$ need not be continuous at the boundary of the well.) To test your knowledge of the steps involved in finding the wave-function, specialize to this case and find the energy eigenstates and eigenvalues using this new boundary condition. Check your answers with the results given on page 172. Be sure you can solve the infinite square well problem completely from memory.

For further practice with these ideas solve problem 5-7 and the first part of 5-8.

6. To gain additional familiarity with the square-well eigenstates, solve problem 5-13. Also calculate the expectation values of the operators in table 4.2 in the states:

a. $\psi_1(x) = N_1 \cos\left(\frac{\pi x}{2a}\right)$

b. $\psi_2(x) = N_2 \sin\left(\frac{\pi x}{a}\right)$

c. ψ of problem 5-13.

Here N_1 and N_2 are normalization constants that you may evaluate if you need them.

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