Relative Probability Densities for Multi-Well Bound States

by Edward Damon

Abstract

It is well established that multi-well bound state systems experience behavior similar to avoided crossings, as degeneracies in the wave function due to identical bound states are avoided by shifting bound state energies corresponding to various wells slightly, creating a familiar set of alternating bands and band gaps, with the bands consisting of a set of bound states that are associated with wells within in the multi well potential. Moreover, the existence of transmission resonances within the multi-peak potential is also well documented, with these transmission resonances occurring when the energy of an incoming wave approaches the energy of one of the bond states of a multi-well potential. However, the exact shape of the wave function, and, thus the probability distribution of the particle represented by the incoming wave is not as well described for a system at a transmission resonance In fact, it is not well known whether the probability distribution of the particle within the multi-peak system is affected by the number of wells within the system. The aim of this paper is to establish the effect of the number of wells on the probability density of a particle, which, appears to be a decaying exponential.

Preliminaries

Let us consider a 1-dimensional system of N identical rectangular peaks surrounded by a region of zero potential (see figure 1 for a visual representation). An incoming wave from infinity to the system can be described by a pure freely traveling wave, which can be represented in a basis of E^ikx and E^-ikx where k represents the wave number of the particle and x is a position co-ordinate. At a transmission resonance, the wave function will approach the state [1,0], as in, the wave function consists solely of a right-traveling wave, i.e. pure transmission. At the left edge of such a system, the wave function will again be a pure scattering state with all of the wave right-traveling [1,0] again. However, inside of the system, the wave cannot be described as a scattering state, as it is bound with a

set of “wells,” similar to a multi-well potential (see figure 2 for a visual representation), but with slightly differing boundary conditions. Instead, the wave function will be a set of sins and cosines, each with some amplitude, as each well can be roughly treated as a single square “well” of finite depth. The natural way to describe this would be to shift to another basis inside of the “multi-well” system, and to solve the Schroedinger equation in this basis. However, a more elegant way to describe this system is to take advantage of a transfer matrix, with with we can represent the state inside each well in terms of our original scattering basis.

Physically, each time the particle passes through a peak, the wave function picks up the transfer matrix, e.g $|\phi(n)\rangle = T^*|\phi(n-1)\rangle$. It is obvious that this transfer matrix is subject to a number of constraints, foremost of which is the fact that the application of N such transfer matrices will return the original wave function, as the particle is in an identical state at either side of the multi-peak potential. Thus, instead of the previous approach, we can instead consider a case in which, instead of picking up a copy of the transfer matrix each time the particle passes through a peak, the particle will lose a copy of the transfer matrix each time it passes through a peak e.g. $|\phi(n-1)\rangle = T^*|\phi(n)\rangle$. Either approach is equally valid, however, for the purposes of this paper, the first approach will be the one used. A further discussion of the exact methodology can be found in the methods and procedures section.

As previously noted, each transmission resonance in the multi-peak system, and, thus, energy chosen for analysis corresponds to a bound state in a multi-well system. Obviously, the wave function for a multi-peak potential does not correspond exactly to the wave function for a multi-well potential, but, it would be likely that some of the symmetry properties of the multi-peak system would be similar to the symmetry properties of a multi-well system. Moreover, the band/ band-gap structure of a multi-well potential should be familiar to solid state physicists, and, to non-solid state physicists, offer an easy foothold to the system under consideration. Therefore, a review of the symmetry properties of the multi-well system is in order.

In a multiwell potential similar to the multi-peak potential involved under analysis in this paper, each bound state in a band can be associated with a certain symmetry in the wavefunction, with lower

energies corresponding to more fundamental symmetries. For example, consider the case of a three well system. Bound states in such a system alternate between even and odd parity, while, at the same time, alternating between even and odd symmetry. A visual example will help to illustrate this point: (insert picture). It's easy to see that each state maintains some level of symmetry, while, at the same time, varying the type of symmetry shown, symmetry, anti-symmetry, and “three-fold symmetry”.

This example also helps to illustrate that the wavefunction does not have to have components in all of the parts of a multi-piece system. The case of anti-symmetry, for example, has a probability density of zero in the middle well. Thus, it seems that examination of the probability density in any particular well as a function of state will only result in confusion; only through an examination of the probability densities across all wells can we fully understand the effect of increasing or decreasing the number of peaks in the system on the probability of finding a particle inside of the system of peaks. Of course, this analysis has been concerned with bound states of a multi-well system, rather than transmission resonances of a multi-peak system, but, an understanding of the simpler multi-well system can only aid in understanding the nature of the multi-peak system. However, the time has come to shift our analysis to the system at hand, the multi-peak system.

Methods and Procedures

As noted in the preliminaries section, the basic tool that will be used for analysis of the multi-peak wave function is the transmission matrix. As noted in Elementary *Quantum Mechanics in One Dimension* (Gilmore, 04) a piecewise constant potential can be described by taking an initial wave function and applying successive transfer matrices to it. In fact, the multi-peak system is one of the examples given of a system which is well-suited to this sort of analysis. However, the challenge of this approach is that, in order to compute the full probability density of a particle inside of the system, one needs to stop after each application of a transfer matrix and integrate the wave function over the region described. A visual representation of the process can be found here: (Insert flowchart).

Calculation of the transfer matrix for each portion of the piecewise potential is fairly

straightforward, following the method laid out in Gilmore 04, however, the transfer matrix, rather than being a 2x2 complex matrix, is instead a 2x2 complex matrix, which is accomplished by transforming into the sin/cos or sinh/cosh set of basis states, depending on if the wavefunction is being evaluated in a valley or a peak.

The integral of the wave function in each region can be performed analytically, however, due to the number of regions to be evaluated, such a step is impractical. Instead, integration over each region is handled via a system of Riemann rectangle While this method introduces errors of second order, this loss of accuracy is small enough not to have a major effect on calculations of the wave functions of interest. Another challenge comes from picking energies at which to evaluate the system. The exact energies that correspond to transmission resonances change as the number of peaks in the system changes, which means, in order to keep examining the behavior of the wave function at a particular transmission peak, the energy of the system must change. As the energy of the system changes, the ratio of the wave function outside to the wave function inside changes, as the wave functions inside the set of barriers look less and less like bound state waves and more and more like freely moving waves.

Thankfully, the effect of energy change on the wave function of the particle inside of the system of peaks has already been characterized. The ratio between the exterior and interior wave function goes as $\exp(\int \sqrt{(m/h^2 * (V-E))}dx)$ (integrated over the entirety of the potential) (Gilmore, Class notes), and, moreover, since the exact probability density of the exterior wave function can be known at a transmission resonance, this effect can be filtered out of calculations, allowing for targeted examination of the effect of peak number of probability density.

The problem remains, of course, of identifying the energies of transmissions resonances. This problem is actually fairly straightforward when cyclic boundary conditions are applied. One computes the transmission matrix for a single unit cell, where a cell corresponds to a pair of peaks and the valley between them, and then computes the traces of this matrix. Then, when (cos 2*pi*k/N) = 1/2(trace), where N is the number of "cells" in the potential and k is an integer that varies between 0 and N-1, we

see a transmission resonance Thus, finding the energy to evaluate the wave function at in order to examine the behavior at transmission resonances can be done quickly and efficiently, if the system is subject to cyclic boundary conditions.

Since this paper is interested in the behavior of the wave function as a result of modifying the number of peaks, rather than the effect of boundary conditions on the wavefunction, it behoove us to choose the boundary condition that makes calculation the simplest Furthermore, the assumption of cyclic boundary conditions has some resonance in the "real world" of physics. Consider the case of a highly energy electron scattering from a metal target, something that is well described by a lattice of N "peaks" with a cyclic boundary condition.

Thus, we have all of the components needed to examine the probability density of the wave function inside an n-peak system with cyclic boundary conditions: the energies to examine the wave function at, how to calculate the wave function in each unit, and how to integrate the wave function once it has been calculated, all of which can be accomplished by a single python program[1]. The only problem with this approach is that we're forced to examine behavior at transmission resonances, and, moreover, are limited to calculating probability densities, rather than true probabilities, however, outside of transmission resonances, the problem rapidly spirals out of control, as the group-theoretic approach of using a transmission matrix no-longer works, and one would need to apply and re-apply the Schroedinger equation in each piecewise part of the potential.

Results

The results of the calculations described above can be neatly summarized on a graph, contained in appendix II. The graph plots the summed probability density of all parts of the well, on the y axis, vs.

1 For the code used in this program, consult appendix I.

the number of peaks, on the x axis. The first portions of the graph are dominated by very sharp swings in the summed value of the probability of finding the particle within the well. This is due to the fact that, for small N, the change in energy between transmission resonances (bound states of the multi-well potential) is very large, so the energy effects dominate the effect (in fact, at N = 4 and 6, there's a large drop in probability as the program finds the resonance at E ~3 (~2 for the case of N = 6), rather than the standard resonance at E ~4.7. However, as the number of barriers increases, the change in energy between any two wells becomes very small, so the dominating effect is the change in the number of peaks.

The total summed probability levels off as we approach N = 50 (the limit of the simulation), however, there remains a slow downward trend. This suggests the effect of increasing N on the summed probabilities seems to a have a roughly exponential dependence, once one factors out the energy effects. This is entirely reasonable, as the particle will not remain bound to the system, and, so, must escape, and, moreover, the size of the system is increasing with N, we would expect the chance of finding the ball in any particular portion of the potential to drop in which a manner. The fact that the probability continues to have a sharp difference between different N's is somewhat disconcerting, and might be the result of a problem in re-normalizing the probability.

Conclusions

The use of transfer matrices in multi-barrier potentials allows for easier, faster, and, above all, simper calculation of the wave function of a particle passing through the potential. However, the effect of adding additional barriers to the potential on the probability density of the wave function inside is somewhat unusual, at least at first glance. However, since for a free particle we can only deal with probability density, rather than true probability, and since the particle must escape the barriers, as we're examining a transmission resonance, the fact that the probability density decays exponentially is less remarkable. However, the need to normalize the probability, and the fact that the exact energy that we can evaluate the system at changes as we introduce additional barriers, since the locations of the transmission resonances change, there are unusual effects which creep in and may cast doubt on the results of this computation.

Further work which examines the change in the probability density through a very large number of peaks would help to confirm or deny the underlying exponential decay that of the probability density. Moreover, a re-write of the code using a higher-order integration technique than Riemann rectangles would help to reduce the error. Finally, an examination of the effect with different boundary conditions would be very useful, as a lot of the “weirdness” in the probability density might be the result of the boundary condition, which effective extends the potential over an infinite space.

Bibliography

Gilmore, R. *Physics 517*. Drexel University Spring 08' Class notes.

Gilmore R. *Elementary Quantum Mechanics in One Dimension.* 2004 Johns Hopkin's University Press.

Griffiths D. *Introduction to Quantum Mechanics (Second edition)*. 1995 Pearson Education Inc.

Appendix I

Program

```
import numpy
import pylab
from math import *
Data = []
N = 1
while  N <=50:
 V = 5.0 #Peak height
 D = 2.0 # Peak Width
 energy = .0001
 L = 6.0 # Well Width
 T = []
 alpha = [0,0]
 beta = [0,0]
 dE = .0001
 E = []
# Transmission matrix of a unit cell
 i = 0
 Trig = 0
 while 1==1:

        k0 = .5125*sqrt(energy)
        k = .5125*sqrt(V-energy)
        matpeak= [cosh(k*D), sinh(k*D)], [-k/k0*sinh(k*D),k/k0*cosh(k*D)]
        matvalley = [cos(k0*L), sin(k0*L)], [-k0/k*sin(k0*L), k0/k*cos(k0*L)]
```

```
        M = numpy.dot(matpeak, matvalley)
        Matrix = numpy.dot(matpeak, matvalley)
        m = 1
        while m < N-1:
                Matrix = numpy.dot(Matrix, M)
                m += 1
        Matrix = numpy.dot(Matrix, matpeak)
        alpha[0] = (Matrix[0][0] + Matrix[1][1])/2
        beta[0] = (Matrix[0][0] - Matrix[1][1])/2
        alpha[1] = -.5*(k0*Matrix[0][1]+Matrix[1][0]/k0)
        beta[1] = .5*(k0*Matrix[0][1]-Matrix[1][0]/k0)
        T = [alpha[0] + alpha[1], beta[0]+beta[1]],[ beta[0]+beta[1], alpha[0] - alpha[1]]
        Tr = T[0][0] + T[1][1]
        #this loop will cycle until we find a transmission resonance
        for m in range(N):
          if abs(.5*Tr- cos(2*pi*m/N)) <= .001:
            Trig = 1
         #print "Found one"
            break
      if Trig == 1: break
        energy += dE
        i +=1
 print energy
#now to calculate the wave functions for each bit
 Initial = [1,1] #wave function is purely right traveling
#WF's are from left to right
```

```
 i = 0
 WF = [[1,0 + 1J]]
 while i< 2*N-1:
  if i%2 == 0:
    T = [cosh(k0*D), sinh(k0*D)], [-k0/k*sinh(k0*D),k0/k*cosh(k0*D)]
  else:
     T = [cos(k*L), sin(k*L)], [-k/k0*sin(k*L), k/k0*cos(k*L)]
  WF.append(numpy.dot(T, WF[i]))
  i += 1
#let's normalize
 check = WF[2*N-1]
 x = check[0] + check[1]
 norm = abs((x.real+x.imag)*(x.real-x.imag))
 i = 1
 while i <= 2*N-1:
          WF[i] = 1/sqrt(norm)*WF[i]
          i +=1
 #print WF[2*N-1]
#alright, now, theoretically, we have some wave functions, time to integrate!
#since they're sin and cos, or sinh and cosh, it shouldn't cause a huge problem, as they don't freak out in
the range we're examining
 i = 1
 Prob = 0
 while i < 2*N-1:
  j = 0
  while j <10:
```

```
    if i%2 == 0:
            x= (WF[i][0]*cosh(k0*j/D))+ (WF[i][1]*sinh(k0*j/D))
           # print  1/D*(x.real +x.imag)*(x.real - x.imag)
            Prob += abs(1/D*(x.real +x.imag)*(x.real - x.imag))
    else:
            y= (WF[i][0]*cos(k*j/L)+ (WF[i][1]*sin(k*j/L)))
            Prob += abs(1/L*(y.real +y.imag)*(y.real-y.imag))

    j +=1
  i+= 1
 #print Prob
 Data.append(Prob)
 N += 1
 print N
pylab.plot(Data)
pylab.show()
```

Appendix II

The Graph