

## Chapter 10.00D

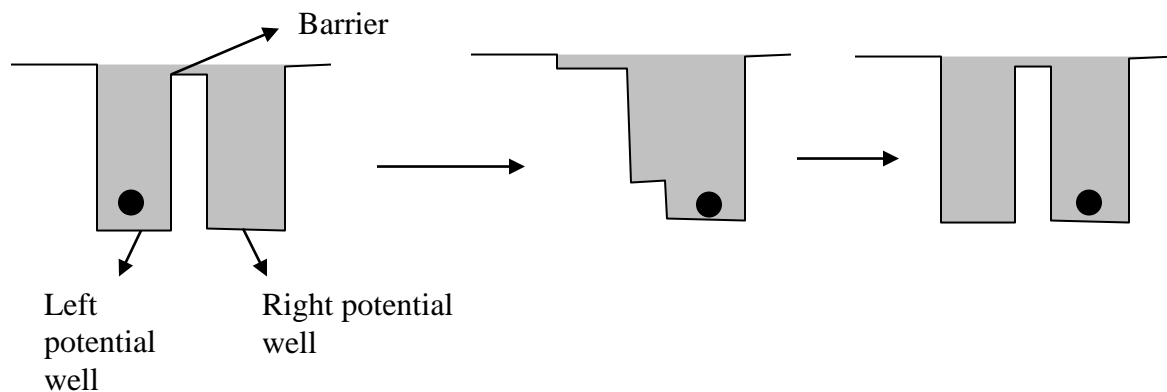
# Physical Problem for Partial Differential Equations Computer Engineering

### Problem Statement

This is the era of nanotechnology. Humans now have the ability to manipulate things in the nanometer range, even single electrons. This has opened up exciting new directions in the design of computer where computations are performed by manipulating single electrons – the ultimate limit in electronic computers. In this problem, we are going to investigate the physics behind such manipulations.

### Problem Formulation

You might recall from your physics class that an electron is neither entirely a particle, as depicted in Figure 1, nor is it just a wave. It exhibits properties of both a particle and a wave (wave-particle duality) and its dynamics is governed by the Schrodinger equation, which is the key equation in quantum mechanics. One should not be daunted by the mention of quantum mechanics. One can look upon this equation as being just a wave equation, like one that can be written to describe water waves, but for the quantum domain. One major difference is that we allow for complex valued wave functions. Without much ado, since the details can be found in most introductory quantum mechanics books, the Schrodinger equation is of the following form



**Figure 1:** Controlling the movement of electron from one potential well to another.

A potential well is a region of space (of nano-meter dimensions) where the energy is locally lower than the surrounding, thereby trapping the electron to stay in that well. The electron can be moved from one well to another by lowering the potential barrier between the cells and increasing the potential of the starting well.

$$i\hbar \frac{\partial \psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x,t) + V(x,t)\psi(x,t)$$

$\psi(x,t)$  is called the **wave function**. It is complex valued and is a function of  $x$  – the space variable and  $t$  – the time variable. This is a 1D wave function. Analogously, we can have 2D and 3D wave functions by introducing the other space coordinates. However, for this problem, we will stick to just 1D. The interesting observation is that the square of magnitude of the wave function at any space-time,  $(x,t)$ , point gives us the probability of finding the electron at that location. Thus  $|\psi(10,2)|^2$  is the probability of finding the electron at location  $x = 10$  and at time  $t = 2$ .

$V(x,t)$  is the **external potential field** that is applied to the electron. It can be used to manipulate the potential wells in our example. Note that it can be time varying. The other constants are  $i$  – the square root of -1,  $\hbar$  – the Planck's constant and  $m$  – the electron mass. Values of these constants can be readily found on the internet. If we fix the spatial dimensions,  $x$ , to be units of angstroms, i.e.  $10^{-10}$  m or 0.1 nanometers, and time to be in the order of femto seconds, that is  $10^{-15}$  seconds, then the Schrodinger partial differential equation can be expressed as

$$i \frac{\partial \psi(x,t)}{\partial t} = -5.7884 \frac{\partial^2}{\partial x^2} \psi(x,t) + 1.5193V(x,t)\psi(x,t) \quad (1)$$

We will solve this partial differential equation for different  $V(x,t)$  forms that capture the raising and lowering of potential wells. To numerically solve the Schrodinger equation, one of the challenges is to maintain the total probability. Since the square of the modulus of the wave function is the probability, its integral over space should be one at all times. We thus have the constraint that

$$\int |\psi(x,t)|^2 dx = 1$$

We have to be careful to enforce this condition when computing the value of the wave function at the next time instant by using finite difference approximation of the time derivative. Typically, we employ the Cayley form to compute the infinitesimal time translations and we solve the spatially discretized problem using the Crank-Nicholson method.

### Worked Out Example

This example is structured to show how the electron can be moved from one potential well to the next by manipulating the external potential field,  $V(x,t)$ . We will transform this external field to guide the electron into the next well. Of course, since an electron is a quantum entity, we cannot talk about its absolute location as we do for particles, but only talk about probability distributions over possible locations represented by the square of the wave function.

We start by defining some primitive functions that we will use to express a family of potential fields as a function of time. Let  $u(x)$  be a pulse shaped function that is one in the range  $-l \leq x \leq l$  and zero elsewhere. Let  $g(x)$  be the exponential function given by

$$\sqrt{\frac{2}{\pi a}} \exp\left(-\frac{x^2}{a}\right).$$

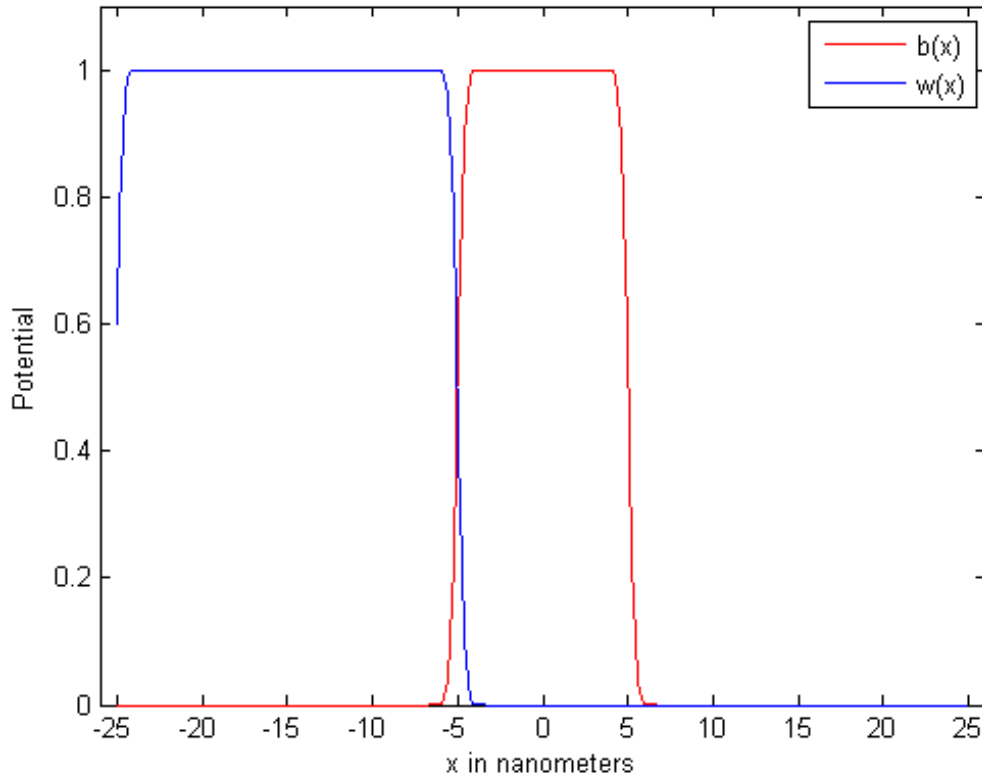
Then, a smoothed version of the pulse,  $s(x)$ , given by  $\int u(y)s(y-x)dy$

(this can be implemented in MATLAB as: `convn(u, g, 'same')`). Using this, we can further define two functions that we will use to characterize the potential at the barrier between the wells,  $b(x)$ , and the potential at the left well,  $w(x)$ . See Figure 1 for the location of the barrier and the left well. Let us denote the domain of  $x$  over which the two potential wells exist to be between  $-L/2$  to  $L/2$ .

$$b(x) = u\left(\frac{x}{0.1L}\right)$$

$$w(x) = u\left(\frac{x + 0.3L}{0.2L}\right)$$

A visual representation of these functions is shown in the Figure 2 for  $L = 50$  and  $a = 2$ . We have two smoothed pulse functions.



**Figure 2:** Plots of the functions  $b(x)$  and  $w(x)$  that are used to construct the overall potential functions.

We will divide our analysis into 8 time intervals, each corresponding to a particular change in the external potential function as captured in the equation below. Each interval is of  $T$  time

units (femto-seconds). The first time interval reflects the initial condition with barrier between the wells held high at  $V_0$  ( $=0.1$  eV in the implementation). In the second time interval, the barrier is slowly (linearly) lowered. In the third time interval, there is no barrier between the wells and the electron is free to move between the wells. The potential at the left well is then raised slowly over  $T$  time units and then held high for  $T$  time units. This will “nudge” the electron into the (right) second well. During the sixth time interval, the barrier between the wells is slowly raised to further nudge the electron into the right well. This is followed by lowering of the left well potential back to zero. And in the final eighth period, the system is restored to the original potential function and the electron now should be in the second (right) well.

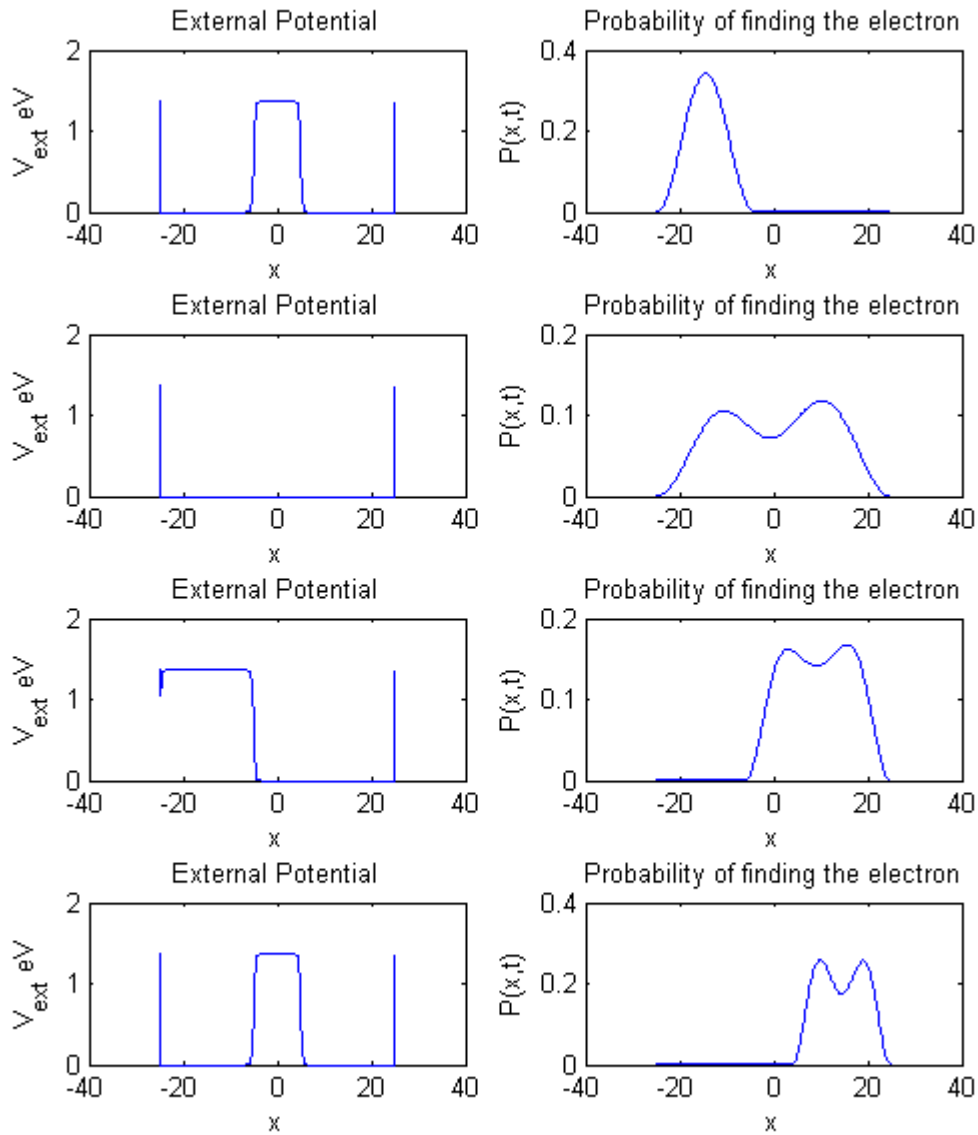
$$V(x,t) = V_0 \begin{cases} b(x) & \text{for } 0 \leq x < T & \text{(barrier held high)} \\ (1 - \frac{t-T}{T})b(x) & \text{for } T \leq x < 2T & \text{(barrier linearly lowered)} \\ 0 & \text{for } 2T \leq x < 3T & \text{(zero barrier)} \\ \frac{t-3T}{T}w(x) & \text{for } 3T \leq x < 4T & \text{(potential linearly raised at left well)} \\ w(x) & \text{for } 4T \leq x < 5T & \text{(left well is held high)} \\ \frac{t-5T}{T}b(x) + w(x) & \text{for } 5T \leq x < 6T & \text{(left well is high, barrier linearly raised)} \\ b(x) + (1 - \frac{t-6T}{T})w(x) & \text{for } 6T \leq x < 7T & \text{(barrier held high and left well is lowered)} \\ b(x) & \text{for } 7T \leq x < 8T & \text{(barrier held high)} \end{cases}$$

We will solve Equation (1) by dividing the time and space coordinates into 0.1 femto-seconds and 1/6 nano-meters (resulting 300 samples over 50 nano-meters along  $x$  – axis). The potential wells are 20nm each and the barrier is 10nm wide. These are some typical dimensions that can be fabricated with current technology. Smaller units of time and space discretization can be chosen, but with increased computational cost. We chose the time period  $T$  to be 500 (femto-seconds), with  $8T = 4000$  femto seconds reflecting a 0.25-Tera-Hz switching clock period. This clock speed is higher than current (year 2008) computer clocks, which are in GHz range. Thus for each time period we have 5000 iterations. We solve the partial differential equation using Crank-Nicholson scheme.

The initial value of the wave function and the boundary conditions are chosen as follows to reflect the occupancy of the left well by the electron and high potential barrier outside the range of  $x$  under consideration. The wave function is normalized ( $c_0$ ) to represent unit probability.

$$\psi_0(x,0) = \begin{cases} c_0 \sin(\pi(x+0.5L)/0.4L) & -0.5L \leq x \leq -0.1L \\ 0 & \text{elsewhere} \end{cases}$$

$$V(-0.5L,t) = V(0.5L,t) = 0.1, \forall t$$



**Figure 3:** Numerical solutions for the probability of finding the electrons at the end of different time periods. We show results for at the end of the first, third, fifth and eighth time period. On the left are the sample external fields at each time period. On the right is the probability of finding the electron, averaged over that time period.

For each time period, we compute the probability of occupancy at a function of  $x$ , but averaged over the time period. Thus,

$$P_{nT}(x) = \int_{nT}^{n+1T} |\psi(x,t)|^2 dt$$

Figure 3 plots these probabilities for some salient time periods. In the beginning, as the probability density function shows, we have the electron in the left well. With the lowering of the well, the probability is smeared over the two wells, denoting the situation that the electron is almost equally likely to be at each well. With the raising of the potential at the left well, the electron is nudged to be mostly at the right well. The probability is further constricted to be over the right well with the raising of the barrier. We are done. The electron is now most likely to be found in the right well.

### Questions and Assignments

1. Study the change in the nature of the solution with different initial shapes of the wave function,  $\psi(x,0)$  .
2. What happens if we remove the smoothing operation that is used to generate the external field profiles?
3. Visualize the wave function (actually the square of the modulus of the wave function) that is computed at each iteration. You will notice how the probability waves are reflecting off the barrier waves.

PARTIAL DIFFERENTIAL EQUATIONS	
Topic	Physical problem for optimization for computer engineering
Summary	A physical problem of manipulating electrons in the design of computers
Major	Computer Engineering
Authors	Sudeep Sarkar
Date	September 14, 2013
Web Site	<a href="http://numericalmethods.eng.usf.edu">http://numericalmethods.eng.usf.edu</a>