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Quantum Simulation of Electron Transport in Arbitrary Barriers

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Abstract— *Due to the pressure on enhancing the power of the processor set by Gordon Moore predicted, the co-founder of Intel, companies such as Intel, Samsung, Taiwan Semiconductor are racing to miniaturise the size of their transistor every two years to compete in the semiconductor market. However, due to limiting factors such as photolithography resolution (limited by diffraction of light), the density of transistor (heat dissipation) and quantum tunnelling, the growth is starting to slow down, as it requires much initial investment to overcome these obstacles.*

This report aims to simulate how the electron behaves during when penetrating a barrier and, confined in a well. The simulation was done using Transfer Matrix Method and Finite Difference Method in MATLAB. There are various uses of quantum well and barriers such as single electron transistor, resonance tunnelling diode, scanning tunnelling microscope, and quantum well light source and cascade laser.

I. INTRODUCTION

As the technology advances, the rate of transistors in a single computer chip is increased by miniaturising the transistor. Gordon Moore, the co-founder of Intel, observed the number of transistors in an integrated circuit doubles every two years. Quantum technology is an emerging field with promising advancement to the field of quantum computer and cryptography but also on solid-state devices (1). Some calculation takes a vastly long time to do by classical computer due to its use binary states whereas quantum computer uses Q-bits, which is a superposition of different states that can make complicated calculation exponentially faster (2).

Quantum mechanics emerged around the time when J.J Thomson discovered the electron using cathode rays and having a sizeable charge-to-mass ratio in 1897. The apparatus comprised of a heated cathode that causes the gas to ionise. The charged particle beam is introduced to an electric field, which causes the beam to be attracted to the positive plate. Robert Millikan, using an oil drop experiment, could determine the charge of an electron by suspending the charged oil drop applying an electric field to oppose the gravitational force. He discovered that the charge of different oil drops was divisible by e, the charge of an electron, 1.6x10-19 C. discovered that the charge of different oil drops was divisible by e, the charge of an electron, 1.6×10^{-19} C. (3)

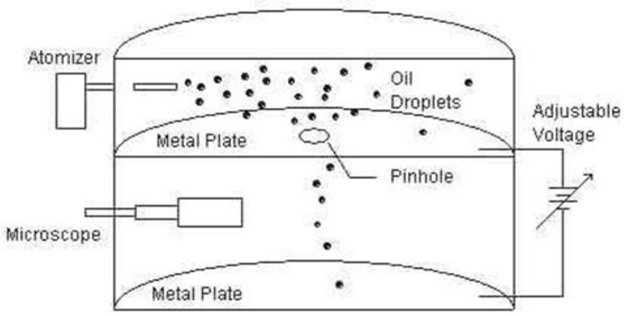

Figure 1: Millikan's oil drop experiment (3)

However, the proposed theory of atom during the early 1900's was Bohr Model, electron orbited the nucleus, and incorporated the idea that electron was a point particle and explain the photoelectric effect where the intensity did not affect ionising whereas frequency did. However, there are various limitation of this model such as; it could not explain the line spectra of complex atoms and why the intensity varies. (4)

A. *Schrödinger equation and wave-particle duality*

Quantum mechanics incorporates the wave-particle duality, which could explain the problems that Bohr model could not. In quantum mechanics particles are treated as a wave with probabilistic nature, diffraction pattern had proven that particles could behave as waves. The electron was fired at thin graphite sheet causing an interference pattern similar to light waves. (5)

Albert Einstein received a Nobel Prize in Physic in 1921, for describing the photoelectric effect. At that time, the classical viewpoint was that ionisation energy of electron was related to the intensity of light but Einstein, with the help of Louis de

Broglie, discovered that energy of light was proportional to frequency and behaved as a stream of discrete wave packets called photons. Alongside
Einstein, Louis de Broglie hypothesis that particle such as an electron can exhibit wave-like behaviour (6).

$$E = mc^2 = \sqrt{p^2c^2 + {m_0}^2c^4}, \therefore p = \frac{E}{c} = \frac{E}{\lambda f} \qquad (1)$$

The energy of the photon is equal to the potential energy plus the kinetic energy, but since the rest mass of the photon is zero, this equates energy to be equal to the product of momentum and the speed of light.

$$\Delta E = hf, \qquad (2)$$

Max Plank postulated that energy had to be discretised at the atomic level; this had to be true to describe the blackbody spectrum. The change of energy between the energy levels is proportional to the frequency of light emitted or absorbed, where h is a constant of proportionality. (7)

$$p = \frac{h}{\lambda} \qquad (3)$$

$$\lambda = \frac{h}{p} = \frac{h}{mv}\sqrt{1 - \frac{v^2}{c^2}} \qquad (4)$$

Louis de Broglie hypothesised that if photons have momentum, then particles also can exhibit a wave-like behaviour. Therefore, a particle such as an electron can have a wavelength, which is inversely proportional to its velocity.

$$p = mv; \quad K = \frac{1}{2}mv^2 = \frac{p^2}{2m} \qquad (5)$$

$$E = K + V = \frac{p^2}{2m} + V \qquad (6)$$

The fundamental postulate of quantum mechanics is the concept of the wavefunction (Ψ), which is a mathematical representation of the quantum state of a system, derived from Schrödinger equation.

$$E\Psi(x) = -\frac{\hbar^2}{2m}\frac{d^2\Psi(x)}{dx^2} + V\Psi(x) \qquad (7)$$

Using conservation of energy, Newton's second law and de Broglie's relationship between momentum and wavelength, Schrödinger was able to merge them into a linear differential equation, which describe quantum mechanical behavior. (5)

B. *Heisenberg Uncertainty Principle*

At the atomic scale, it is impossible to describe particles specific events with absolute precision. The uncertainty is not due to the limitation of quantum mechanics but rather the probabilistic nature of particles.

The uncertainty is not due to the limitation of quantum mechanics but rather the probabilistic nature of particles.

$$(\Delta x)(\Delta p_x) \geq \frac{\hbar}{2} \qquad (8)$$

Whenever a measurement is taken, more precisely the position of a particle is known, smaller Δx, the precision of its momentum is going to decreases, larger Δp_x and vice. Therefore, for quantum particles, it is impossible to measure its position (Δx) and its momentum (Δp_x) simultaneously. (5) (8)

$$(\Delta E)(\Delta t) \geq \frac{\hbar}{2} \qquad (9)$$

The above equation is the second form of Heisenberg uncertainty principle, and it states that the uncertainty measurement in energy (ΔE) will be related to uncertainty in time (Δt).

$$\int_{-\infty}^{\infty} P(x)dx = 1 \qquad (10)$$

Due to the uncertainty principle, probability density function can be used to find its relative likelihood of finding a particle.

C. *Wave Function*

Quantum mechanics considers the wave-particle duality of nature, as it describes a particle as waves. Louie de Broglie concluded that momentum of a particle is related to its wavelength so in quantum mechanics a particle is described using a wave function ($\Psi(x, t)$) and it is a function of position and time. (5)

$$\Psi(x, t) = A\, e^{i(kx - \omega t)} \qquad (11)$$

$$\int_{-\infty}^{\infty} |\Psi\Psi|^2 dx = 1 \qquad (12)$$

For a wave function to be useful, it must satisfy specific constraints such as, it must be a solution to Schrödinger equation, the wave function must be continuous, and it must be normalized. Under the normalized condition, the probability of finding a particle between infinity and –infinity is always equal to one. (6)

II. Theory

A. *Quantum Well*

The allowed quantised energy states can be solved by solving the Schrödinger equation; these discrete energy level corresponds to the electrons orbitals.

$$V(x)\begin{cases} 0 & for\ 0 < x < L \\ \infty & otherwise \end{cases} \qquad (13)$$

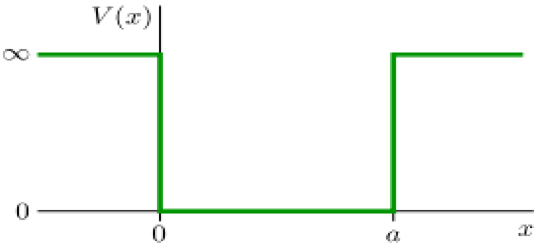

Figure 2: Infinite Potential Well (10)

Particle in a box model is used to describe how a particle behaves when it is surrounded by an impenetrable barrier, for this case an electron confined to a one-dimensional potential rigid box of width (L). The particle can move along the width, and the collision with the walls are perfectly elastic. (9)

The allowed energies of the electrons can be obtained by solving the Schrödinger equation must be solved. The potential energy at $V(0 < x < L)$ is equal to zero otherwise potential energy at $V(x < 0)$ and at $V(x > L)$ is equal to infinity. (9) (10)

$$\Psi(x) = A\, e^{ikx} = a\sin(kx) + b\sin(kx) \qquad (14)$$

So, at x = 0 and x = L, only $a\sin(kx)$ satisfy the boundary conditions if k=$\frac{n\pi}{L}$ where n is a positive integer.

$$\Psi(x) = a\sin\left(\frac{n\pi}{L}x\right) \qquad (15)$$

$$E_n = \frac{\pi^2 n^2 \hbar^2}{2mL^2}, \qquad (16)$$

$$\lambda_n = \frac{nL}{n} \qquad (17)$$

The above equation shows the discrete energy level; only specific values of energy can be occupied.Also, when the wave function is normalized, the probability of finding the electron at the energy levels can be visualised. (6)

$$\int_{-0}^{L} |\Psi\Psi|^2 dx = 1\ ;\ a = \sqrt{\frac{2}{L}} \qquad (18)$$

$$|\Psi(x)|^2 = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right) \qquad (19)$$

B. *Quantum Tunnelling*

In the fields of quantum mechanics, particles such as electrons can penetrate a potential barrier into a region that is forbidden in the viewpoint of classical mechanic.

A particle of mass (m) with no potential energy moving with kinetic energy (E), when it interacts with a potential barrier (E<V) the particle will have a specific probability that it will penetrate through.

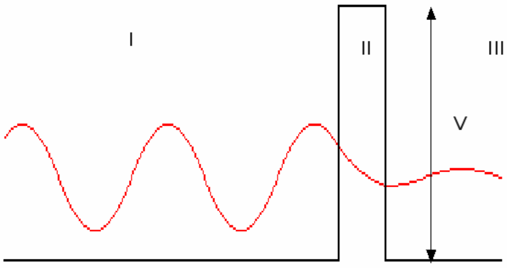

Figure 3: Potential Barrier of height V (11)

$$Region\ I : \Psi_1(x) = Ae^{ik_0x} + Be^{-ik_0x} \qquad (x < 0) \qquad (20)$$

$$Region\ 3 : \Psi_3(x) = Fe^{ik_2x} + Ge^{-ik_2x} \qquad (x > L) \qquad (21)$$

$$where\ \ k_0 \begin{cases} x < 0 \\ L < x \end{cases} = \sqrt{\frac{2mE}{\hbar}} \qquad (22)$$

A free particle can be represented by the wave equation Ψ(x). At region 1: V(x) = 0, the solution to this problem is sinusoidal waves that are travelling in a different direction. A e^{ik_0x} represents the forward travelling wavefunction whereas Be^{-ik_0x} is the reflected wavefunction from the barrier. Thus, at region 3, Fe^{ik_0x} is the transmitted wave that managed to tunnel through the barrier. (6)

$$Region\ 2 : \Psi_1(x) = Ce^{ik_1x} + De^{-ik_1x} \quad (0 < x < L) \quad (23)$$

$$where\ \ k_1 = \sqrt{\frac{2m(E-V)}{\hbar}} \qquad (24)$$

At region 2, the potential barrier amplitude compared to the particle kinetic energy (V>E), resulting in k being an imaginary number. Therefore, resulting in the product of imaginary term being a negative one, Ce^{-k_1x}. As the wavefunction travel through region 2, it decreases exponentially. (6) (11)

$$T{+}R = 1 \qquad (25)$$

The transmission coefficient represents the ability of the particle to penetrate the barrier. The probability of particles that tunnel through the potential barrier (T) and the probability of particles that reflected off the barrier (R) should always be equal to one. (6)

III. SIMULATION METHOD

A. *Finite Difference Method*

Finite difference Method can be used to approximate differential equation for complex geometrical shaped wells. Schrödinger equation can be used to solve the eigenvalue problem as resonating systems produces distinct patterns has eigenmodes. (12)

$$Ax = \lambda x \qquad (26)$$

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right]\Psi(x) = E\Psi(x) \qquad (27)$$

In quantum mechanics, eigenvalue (λ) represents the energy levels (E_n) of the bound state in a potential. Eigenfunction (x) is represented by the wavefunction $\Psi(x)$, and the operator (A) represents the Hamiltonian operator ($\widehat{H}$). (12)

$$\left.\frac{d^2\Psi(x)}{dx^2}\right|_{x=x_n} = \frac{\Psi(x_{n+1})-2\Psi(x_n)+\Psi(x_{n-1})}{l^2} \qquad (28)$$

$$E\Psi(x)_n = -\frac{\hbar^2}{2ml^2}[\Psi(x_{n+1}) - 2\Psi(x_n) + \Psi(x_{n-1})] \qquad (29)$$

The finite-difference approximation is used to discretise and solve the Schrödinger equation for the time-independent case. By using this method, the solution can be solved numerically along the length (L) where l is the spatial interval spacing.

$$E\boldsymbol{I}\overline{\Psi} = \widehat{H}\overline{\Psi} \qquad (30)$$

The approximate solution to the Schrödinger equation can be represented in a matrix form where $\overline{\Psi}$ is the diagonal components of the wave function (Ψ), and $\boldsymbol{I}$ is the identity matrix. To solve for complex potential well, V(x) needs to be diagonalised and then added to the Hamiltonian operator. (12)

B. *Transfer Matrix Method*

Transfer matrix method (TMM) can be used to calculate the probability of a particle tunnelling through a potential barrier; successive steps are needed for approximating an arbitrary potential barrier. (13)

$$\Psi_1(x) = \begin{pmatrix} e^{ik_0x} & e^{-ik_0x} \end{pmatrix}\binom{A}{B} = \begin{pmatrix} e^{ik_0x} & e^{-ik_0x} \end{pmatrix}\emptyset_1 \qquad (31)$$

The general solution of the Schrödinger equation can be represented in a vector dot product form for each region. For the above solution, the coefficient vector ($\emptyset_1$) represent the wavefunctions in the region one. (13)

$$A + B = C + D \qquad (32)$$

$$ik_0A - ik_0B = ik_1C + ik_1D \qquad (33)$$

The boundary condition states that the wave function must be continuous at x = 0.

$$m\binom{A}{B} = n\binom{C}{D} \qquad \therefore \binom{A}{B} = m^{-1}n\binom{C}{D} \qquad (34)$$

$$\emptyset_1 = \frac{1}{2}\begin{pmatrix} 1+\frac{k1}{k0} & 1-\frac{k1}{k0} \\ 1-\frac{k1}{k0} & 1+\frac{k1}{k0} \end{pmatrix}\binom{C}{D} = d_{12}\emptyset_2 \qquad (35)$$

The above equation can be expressed in matrix notation and taking the inverse yields the coefficient vector $\emptyset_1$ where d_{12} is known as discontinuity matrix where it connects the coefficient vector of region 1 and region 2. (13)

$$\emptyset'_2 = d_{21}\emptyset'_3 \qquad (36)$$

The boundary condition also states that wave function must be continuous at x=L. The discontinuity matrix d_{21} takes the same form as d_{12} but with change, the indices $\frac{k1}{k0}$ to $\frac{k2}{k1}$.

$$\Psi_2(x) = \Psi'_2(x-L) \qquad (37)$$

$$\emptyset_2 = \begin{pmatrix} e^{ik_1L} & 0 \\ 0 & e^{ik_1L} \end{pmatrix}\binom{C'}{D'} = p_2\emptyset'_2 \qquad (38)$$

Assuming there is no reflected wave in region 3, G= 0, transmission and reflection coefficients are given by the equation above.

IV. Result

A. *Quantum Well*

The amplitude of the probability density function ($|\Psi\Psi|^2$)is scaled down to 0.1, as the width of the well approach zero the amplitude goes towards infinity.

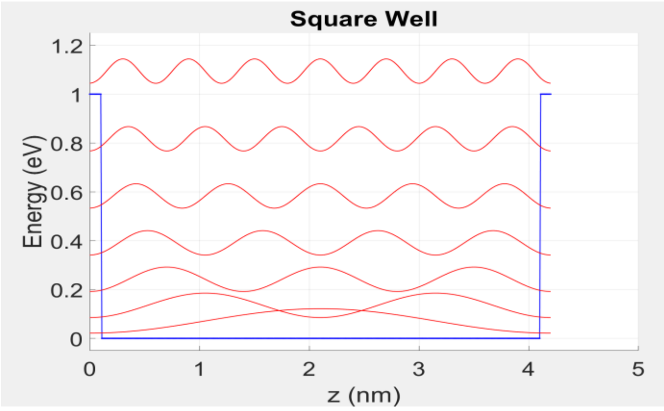

Figure 4: Energy Level of Electron on Square well, height of 1eV and width of 4nm

Figure 4 shows the discrete energy level obtained by solving the Schrödinger equation through finite difference method. The probability density function also shows the likelihood of finding an electron along the width of the well. The lowest energy state (E_0) occurs when n= 1 and has a value of 0.0233eV

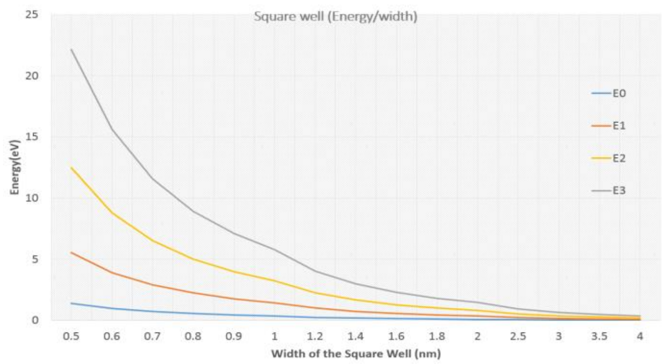

Figure 5: Energy Levels n = (1 to 4) against the width of the square well

The graph, Fig. 5, was obtained from the same Square well shown on Fig. 4 but with increasing the width of the barrier from 0.5nm to 4nm. This graph shows the discrete energy of the wave function beginning to converge exponentially as L increases. Thus, as the width increases the number of energy level increases rapidly.

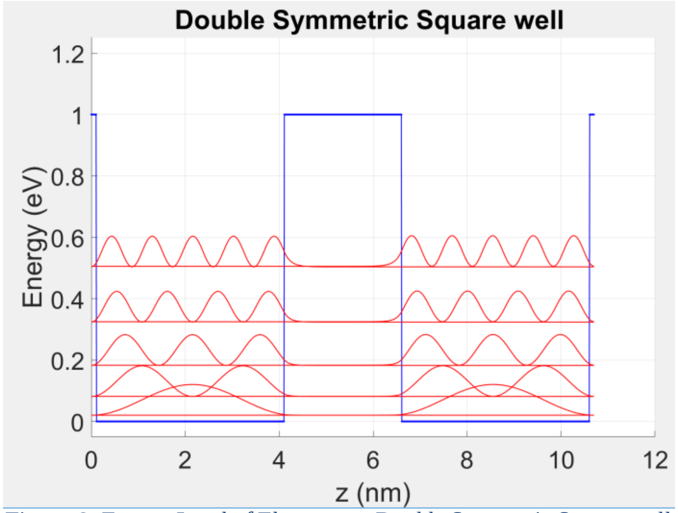

Figure 6: Energy Level of Electron on Double Symmetric Square well, height of 1eV, width of 4nm and the barrier region width of 2.5nm.

Figure 6 shows how electron behave under double symmetric square well. In this case, a potential barrier separates the wells where the pairs of wavefunctions have very similar energy. The value of E_0 and E_1 are 0.0203eV and 0.0204eV respectively whereas E_2 and E_3 are 0.0813eV and 0.0816eV respectively.

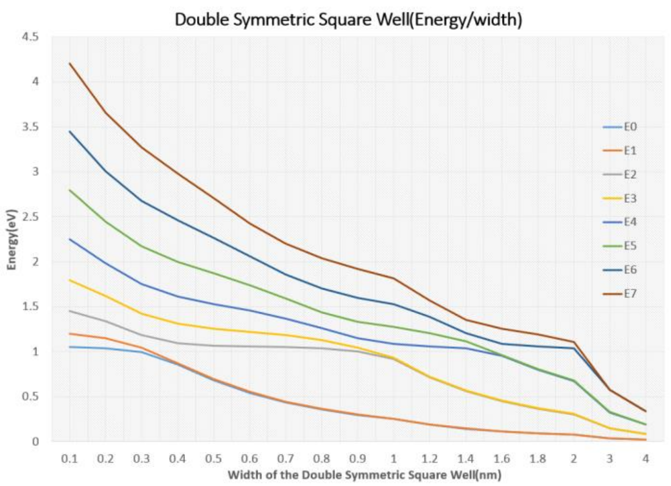

Figure 7: Energy Levels n = (1 to to 8) against the width of the Double Symmetric Square well

The graph, Fig. 7, obtained from the double symmetric square well, shown in Fig. 6, but with increasing the width of the barrier from 0.1nm to 4nm. This graph shows the discrete energy of the wavefunction beginning to converge exponentially as L increases but when the discrete energy is less Then the barrier height (E_n<1eV), E_0 and E_1 beings to converge (energy is very similar), similar case for E_2 and E_3 and so on.

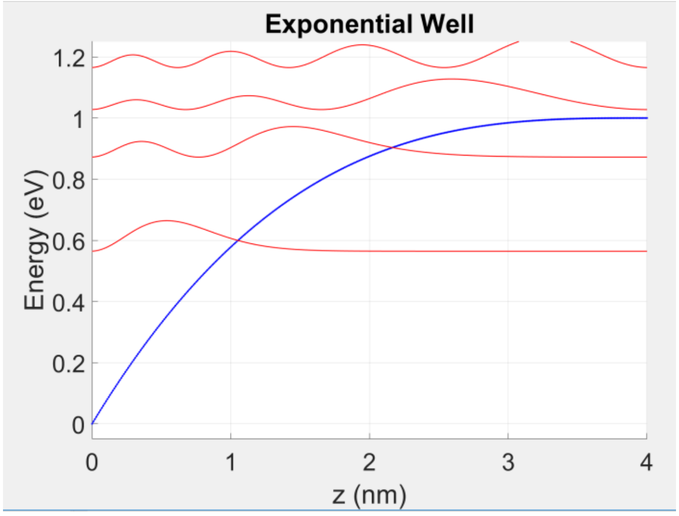

Figure 8: Energy Level of Electron on Exponential well, height of 1eV and width of 4nm

Figure 8 shows how electrons behave under exponential well (V0=$-a(1-e^{-z})$ and its discrete energy level. As seen in the graph, the probability of finding an electron is higher near the well and barrier interface. The lowest energy state (E_0) has a value of 0.564eV and E1 has a value of 0.872eV.

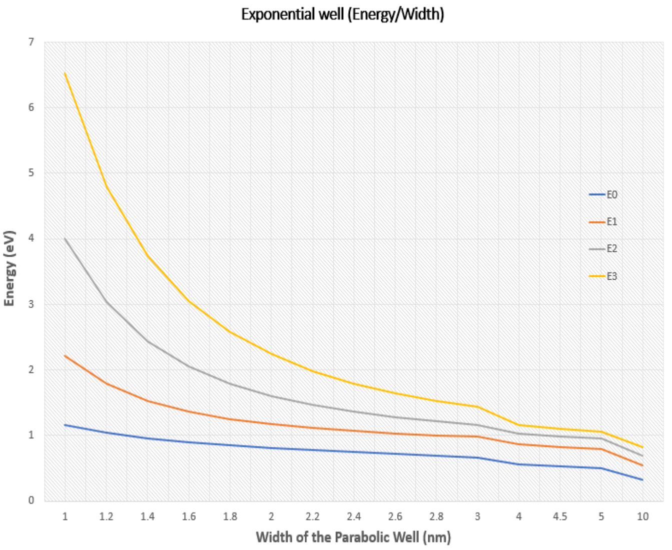

Figure 9: Energy of the wave function n = (1 to 4) against the width of the Exponential well

The graph in Fig. 9 shows discrete the energy of wavefunctions exponentially beginning to converge as width is increased. The graph is comparable to Fig. 5, but the rate of change happens at a slower rate.

B. ***Quantum Tunnelling***

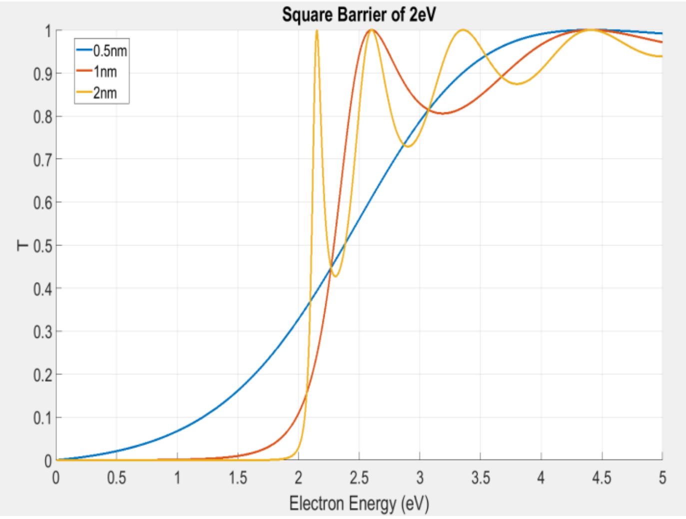

Figure 10: Transmission of electrons vs Energy of Electron on Square Barrier of height of 2eV

Figure 10 shows the dependence of transmission coefficient (T), on electron incident energy when tunnelling through a square barrier of 2eV with various thickness of 0.5nm, 1nm and 2nm. When the barrier thickness is at 2nm, the first peak tunnelling happens at 2.125eV whereas for 1nm and 0.5nm the peak tunnelling happens at 2.603eV and 4.379eV respectively. Even when the electron energy is lower than the barrier (E<2eV) there is a probability that electron can penetrate through, at 0.5nm barrier width electron with 1eV has a transmission coefficient of 0.068.

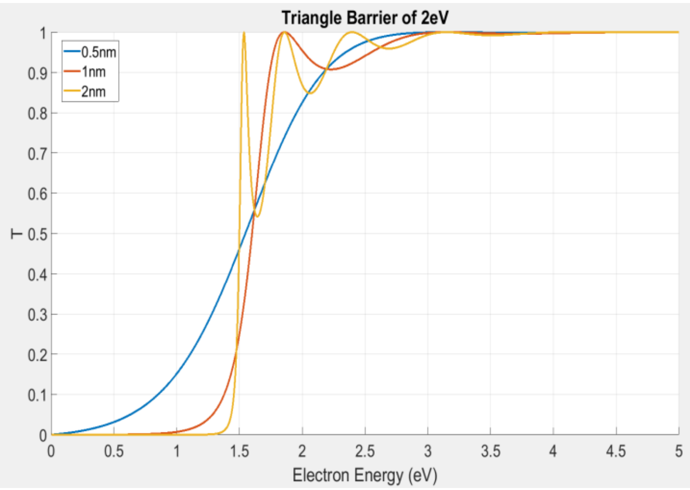

Figure 11: Transmission of electrons vs Energy of Electron on Triangle Barrier of height, Vb= (-x/2) +2

Figure 11 shows the dependence of transmission coefficient (T), on electron incident energy when tunnelling through a triangle barrier, peak height of 2eV with various thickness of 0.5nm, 1nm and 2nm. The first maximum tunnelling occurs at 1.537eV, 1.857eV and 3.098eV at 2nm, 1nm and 0.5nm respectively.

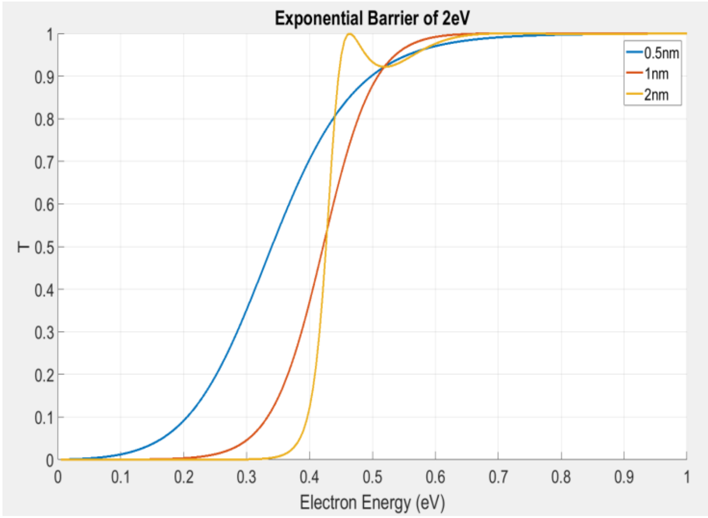

Figure 12: Transmission of electrons vs Energy of Electron on Exponential Barrier of height, Vb= 2(e^ (-5x))

Figure 12 shows the dependence of transmission coefficient (T), on electron incident energy when tunnelling through an exponential barrier, peak height of 2eV with various thickness of 0.5nm, 1nm and 2nm. The first maximum tunnelling occurs at 0.466eV, 0.7eV and 1.161eV at 2nm, 1nm and 0.5nm respectively. The average barrier height is around 0.4eV as the rate of transmission per incident energy happens around that energy.

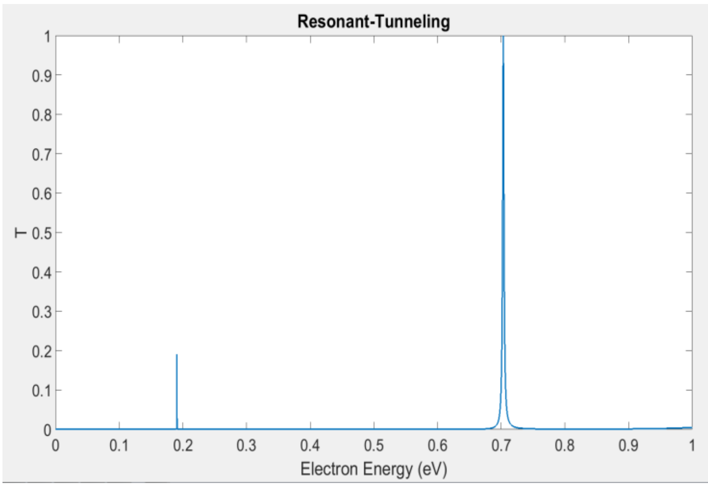

Figure 13: Transmission of electrons vs Energy of Electron on Double Square Barrier

Figure 13 shows the dependence of transmission coefficient (T), on electron incident energy when tunnelling through a double barrier structure, height of 1eV with various thickness of 1nm. At 0.1907eV and 0.7033eV the tunnelling coefficient are 0.191 and 0.9993 respectively.

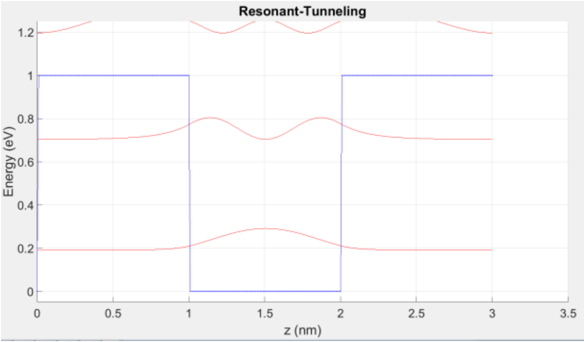

Figure 14: Energy Level of Electron on Double Symmetric Square barrier, height of 1eV, width of 1nm and the well region width of 1nm.

Figure 14 shows how electron behave under double square barrier. In this case, a potential well separates the barrier; the well allows only discrete energy levels, E_0 and E_1 are 0.1907eV and 0.7039 eV.

V. Discussion

The results obtained coincides with the theories and describes how the electron behaves at an atomic scale. The discretized energy levels explain the line spectra as each energy level corresponds to the different wavelength of light. Whereas the tunnelling coefficient is non-zero even during electron energy being less than the barrier energy explain the quantum-tunnelling phenomenon.

A. *Quantum well*

For the one-dimensional case of a particle in a well, the result shows that the energy levels of the particle confined in the well is discrete. Instead of a continuous energy level described by classical viewpoint, the electron in the well can only have certain discrete energies thus energy is quantized as shown in Fig. 4, 6 and 8. The solution for wavefunction in a well are standing waves, equation 15, that are trapped between the impenetrable walls and integer number of half wave exist per energy level.

Due to Heisenberg uncertainty principle the ground state, lowest energy level (E_0), is not equal to zero. For a particle in a well of width L, the uncertainty in position Δx is less than or equal to L. The localization of the particle in the well leads to a greater uncertainty in momentum (Δp) thus the momentum is not equal to zero resulting in a non-zero energy. (5)

As seen in Fig. 4, 6 and 8, the energy level at the well region is discretized, and for each allows En, there is a corresponding density function $(|\Psi\Psi|^2)$. As n increases the number of antinodes increases so the location of finding an electron at that given energy increases. This due to the specific electron energy and the probability density corresponding to each wavelength. The wavelength for any given n is given by equation 17, so as n increases by one the wavelength decreases by a half.

The energy interval increases corresponding to increase in n, in a square well, energy per n increment is equal *to* $E_{n-1} = n^2E_0$ where E_0 is the ground state energy. The ground state energy E_0 at 4nm is 0.02327 and the expected E_1 is 4*E_0, there was 1.53 x10^{-5} which is caused by finite-difference approximation or the resolution.

In a square well, when the length decreases in the well by a factor of two (L/2), the energy in the well will be increased by four. This is because of the energy of the well is proportional to the inverse of the width (L) squared, this can be seen in the graph 5. Whereas on the exponential well, Fig. 8, the width increases at a rate of $L = 1 - e^{-x}$, so at lower values of n, the energy level is very high compared to the square well.

At L= 4nm and Vb =1eV, the ground state energy at n=1, it is 0.564eV for exponential well whereas on the square well it is 0.023eV. Due to the width of the exponential well increasing as when moving along the z-axis, this causes the ground state energy to increase by significantly compared to the square well. This results in fewer allowed energy level, at L=4nm the exponential well only has two allowed energy state whereas square well has six.

The double square well energy levels, Fig. 6, is similar to the values of the square well but comes with pairs of energy levels, which are very similar, but not the same. At L=4, E_0 and $E_1$are 0.0203eV and 0.0204eV whereas E_2 and E_3 are 0.0813eV and 0.0816eV respectively in the double square well compared to square wells energy level E_0 and E_1 is 0.0232eV and 0.0931eV. The pair of energy level, one is an even parity (lower energy), and the other is odd parity (higher energy), the odd and even parity energy level are very similar, but probability density function is reflected around L/2. This can be seen in Fig.19 due to the triple barrier structure, which has two well, during resonance the pairs of energy level allows electron to pass through.

Pauli Exclusion principles state that no two electrons can occupy the same quantum state. Therefore, at the double square wells, lowest energy level, an electron cannot exist in both E_0 and E_1 on the same well so when E_0 is occupied in left well E_1 of right well will be occupied and, vice versa. After some time, the electron will tunnel through the barrier into the other well. (14) (5)

$$t = \frac{\pi\hbar}{E_0 - E_1} \tag{39}$$

The above equation shows the time it takes for an electron to tunnel from one well to the other well. As the width of the barrier increases the change in energy level Δ $(E_0 - E_1)$ will decrease thus resulting in time it takes for an electron to tunnel through the barrier to increase.

As the width of the material increases, energy levels will begin to converge with minimal intervals causing it form energy bands that explain the conduction bands and valence bands that occur in bulk material. An electron can be excited to a higher energy state, providing that the higher energy level has free space to be occupied, this is known as excitation. The electron can de-excite back to the original position and conserve the energy the change of energy is given off as heat or as photon depending on indirect and direct bandgap. (14)

In a semiconductor, there are bandgap separating the valance and conduction band when holes are introduced to the semiconductor lattice; electron form conduction band can combine with holes in valence band thus releasing photon if it is a direct bandgap. If the well in conduction band has a large width, it will produce wide ranges of light corresponding to the sum of energy levels in the well and the band gap.

One way to alter the wavelength of light is by decreasing the wells width, as it discretized the energy level and limit the number of energy levels, thus resulting in the production of a specific wavelength of light with high intensity. Quantum Well can be used to create a particular frequency of an electromagnetic wave with high intensity compared to conventional LED or LCD, and this can be used in display technology as it reduces power consumption, increases colour accuracy, has a higher resolution, and comparing to OLED it does not degrade over time. It can also be used to make a spectrometer that can be used to identify the bandgap of a sample to see what it consists of. (1)

Quantum cascade laser is made from series of coupled quantum wells separated by superlattices, the energy of a photon is much lower than a direct bandgap semiconductor laser. This is due to the excitation and de-excitation occurs within conduction inter-subband quantum well states. Due to subband energy being lower, this enables the device to generate THz radiation (300 GHz to 3THz), this range of frequency can be used in medical imaging and communications. (8)

B. *Quantum Tunnelling*

For the one-dimensional case of particle tunnelling through a barrier, the tunnelling probability is obtained by solving Schrödinger equation by keeping the width constant and varying the incident energy. When the energy of the incident electron is less than the height of the barrier (0<E<V), in the classical viewpoint, the particle should be reflected (R=1), but as seen on Fig. 10, there is a probability of electron tunnelling through the barrier.

$$T = \frac{1}{1+\left(\frac{k_0{}^2+k_1{}^2}{2k_0k_1}\right)^2 sinh^2(2k_1L)}, \quad E < V \qquad (40)$$

Maximum tunnelling in the region E<V (40), occurs when $sinh^2(2k_1L) = 0$, so decreasing the width (L) and decreasing k_1, which can be done by increasing the incident energy of the electron. For a large width barrier, the probability of electron tunnelling through the barrier at E<0 is very low. (6)

$$T = \frac{1}{1+\left(\frac{k_0{}^2-K_1{}^2}{2k_0K_1}\right)^2 sin^2(2K_1L)}, \quad E > V \qquad (41)$$

$$K_1{}^2 = -k_1{}^2$$

For the case when the incident electron energy is higher than the barrier, in the classical viewpoint, all the particle should pass through (T=1), but as seen on Fig. 10, 11 and 12, the maximum tunnelling occurs when $sin(2K_1L) = 0$. Therefore, the peak transmission coefficient occurs when$2K_1L = \pi n$, at certain "resonance" energies whereas minima occurs at $2K_1L = (n + \frac{1}{2}\pi)$, n being a positive integer. This shows that there is some reflection even when the energy of the electron is higher than the height of the barrier, over-barrier reflection (6)

Figure 10, when the width of the barrier is 2nm the electrons first maximum transmission happens at a high gradient at 2.125eV, then it starts to oscillate due to the k_1 being negative. However, at lower width, 1nm and 0.5nm there are fewer oscillations, but the gradient is lower causing the electron to tunnel through even when the incident energy of the electron is lower than the square potential barrier. At these widths, the first peak in transmission coefficient occurs when incident energy is higher than the square potential barrier, 2.603eV and 4.379eV for a width of 1nm and 0.5nm respectively.

However, most of the transmission coefficient increases on the triangle and exponential barriers, Fig. 11 and 12 occurs around 1.5eV and 0.4eV respectively. This is due to the average barrier energy being lower than the peak. For the triangle barrier (11), the oscillate decreases faster compared to the square barrier whereas the exponential potential barrier almost has no oscillate, the amplitude is minimal.

Fig. 13 and 14 show how electrons behave in a double barrier structure, transmission coefficient peak when the incident electron energy matches the confined energy level of the well. The ground-state energy (E_0) occurs at 0.1907eV, in Fig. 14 the first peak of 0.191 in transmission coefficient occurs in 0.1907eV. The second peak of 0.9993 occurs when the incident electron energy is 0.7033eV whereas E_1 has a value of 0.7039 eV. Factors causing the minor difference in energy are the different approximation method and resolution. The first peak as seen on Fig.18 is higher (T= 0.9674), this was due to increases data point from 10,000 to 100,000 which took 10 minutes to simulate.

In the semiconductor industry, quantum tunnelling has caused various problems, as the transistor is scaled down, decreasing the width of the gate to increase processing power. If the tunnelling is quite significant, the electron will tunnel through regardless of the barrier caused by the gate; the transistor would not operate as a switch.

The properties of tunnelling can be used in numerous ways such as scanning tunnelling microscope, which consists of a sharp tip (few nm in width). A high voltage is applied to the tip and a conductive sample, the tip hovers on top of the sample so that tunnelling occurs. By using a feedback system and moving the tip to maintain a constant tunnelling current, a detailed map of samples surface can be produced. (5)

The property of resonance tunnelling can be used as a diode, where tunnelling occurs only during resonance when the energy of the particle is lower than the barrier height (E<V). When the energy of the electron matches the confined energy level of the well, there is a spike in transmission, but in other regions, it is close to zero. By controlling the difference in the height of the two barriers, the position of the confined energy levels of the well can be sifted causing resonance even if the energy of the electron remains a constant. (15)

This property can also be used to create a single electron transistor where a barrier is surrounding a quantum dot; Coulomb blockade takes effect, due to this it only allows a single electron to pass through resulting low power consumption and excellent scalability. (6)

VI. Conclusion

This report investigates how electron transports through an arbitrary barrier and well. Two different simulation method was used, finite difference method and transfer matrix method which was used to approximate the solution for the quantum well and barrier problems.

Quantum well can be used to create a particular frequency of light by altering the confined energy levels, which is useful for display technology, communication and medicine. Quantum cascade laser can produce frequencies that can cover the THz gap, as the energy of conduction inter-subband is much lower than the semiconductors band gap.

Quantum tunnelling becomes a problem as the width of the barrier begins to decreases. Tunnelling is problematic for the semiconductor industry due to the size of the transistor decreases; quantum tunnelling occurs thus there to be a size limitation. Although the property of tunnelling can also be used in various application such as imaging (STM) and active electronic components such as transistor and diode.

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VIII. References

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IX. APPENDIX

A. Finite Difference Method

```
FDM =(-2)*diag(ones(1,Nz)) + (1)*diag(ones(1,Nz-1),-1) + (1)*diag(ones(1,Nz-1),1);
FDM=FDM/dz^2;

H = -hbar^2/(2*me*Mass) * FDM + diag(V0*e) ;

H = sparse(H);
[psi,Energy] = eigs(H,n,'SM');
E = diag(Energy)/e ;
E=real(E);
```

Figure 15: Codes for FDM

B. Transfer Matrix Method

```
for r = 1:3;
    for n = 1:N;
        k0 = sqrt(2*m*E(n))/hBar;
        k1 = sqrt(2*m*(E(n) - V(n)))/hBar;
        k2 = k0;

        D12 = 0.5 * [(1+k1/k0) (1-k1/k0); (1-k1/k0) (1+k1/k0)];
        P2 = [exp(-i.*k1.*L(r)) 0; 0 exp(i.*k1.*L(r))];
        D21 = 0.5*[(1+k2/k1) (1-k2/k1); (1-k2/k1) (1+k2/k1)];

        Q = D12 * P2 * D21; %Transfer Matrix

        AP3 = 1/Q(1,1);
        AP1 = Q(2,1)*AP3;

        T(n) = abs(AP3)^2; %Transmission probability
    end
```

Figure 16: Codes for TTM

C. Extra

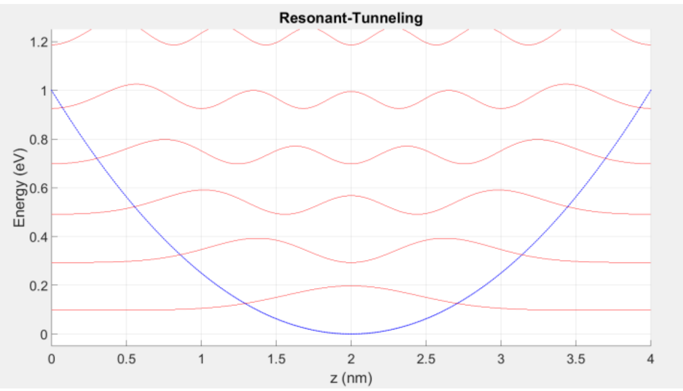

Figure 17: Energy Level of Electron on Parabolic Well, height of 1eV and width of 4nm

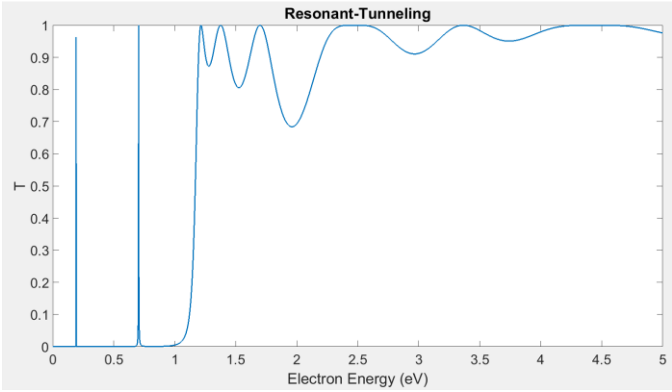

Figure 18: Similar to Fig.13, Transmission of electrons vs Energy of Electron on Double Square Barrier from 0 to 5eV

Double square barrier of 1 eV and data point of 100,000.

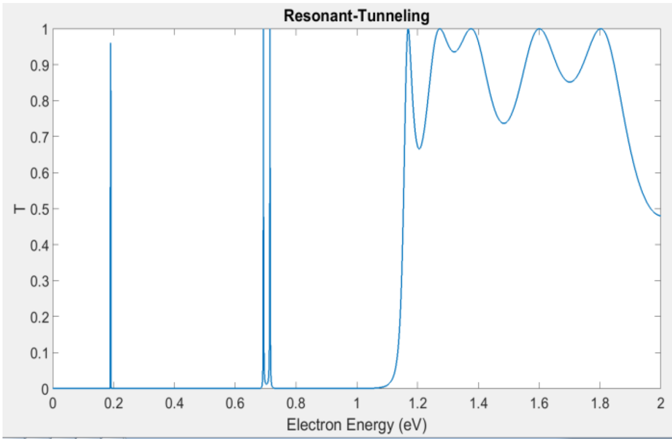

Figure 19: Similar to Fig.13, Transmission of electrons vs Energy of Electron on Triple Square Barrier from 0 to 2eV

Triple square barrier of 1 eV and data points of 100,000