ELECTRON TUNNELING

IN THE

TIGHT-BINDING APPROXIMATION

by

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ABSTRACT

In this thesis, we treat tunneling similar to a scattering problem in which an incident wave on a barrier is partially transmitted and partially reflected. The transmission probability will be related to the conductance using a model due to Landauer. Previously tunneling has been treated using a simple barrier model, which assumes the electron dispersion is that of free electrons. In this model it is not possible to investigate tunneling in the gap between a valence band and a conduction band. We shall remedy this limitation by using the tight-binding model to generate a barrier with a gap separating a valence band and a conduction band. To do this, we constructed a model consisting of semi-infinite chains of A atoms on either side of a semi-infinite chain of B-C molecules. The B-C chain has a gap extending between the onsite energy for the B atom and the onsite energy for the C atom. Tunneling through the gap has been calculated and plotted. We present exact closed form solutions for the following tunneling systems: (i) A-B interface, (ii) A-(B-C) interface, (iii) A-B-A tunnel barrier, (iv) A-(B-C) interface with the orbitals on B having *s*-symmetry and those on C having *p*-symmetry, (v) A-(B-C)-A tunnel barrier.

DEDICATION

To my beloved, Nancy, who has changed my life for the better in ways I could not have fathomed. You are my raison d'être. This is the culmination of love and teamwork. I love you.

To my mother and father, Ronald and Devera, I want to say 'thank you' for a lifetime of inspiration, guidance, and support. I tend to do what I want but your teachings made sure I wanted the best and knew how to work for it.

To my grandparents, Georgia, Iradell, and Willie, you made everything better.

To my siblings, Joshua, LaShonda, and LaTanya, your respect means everything to me. I always wanted to provide a good example for you.

To Kendrick King Jr., you are truly a great person to know and love.

LIST OF ABBREVIATIONS AND SYMBOLS

μ_1	Electrochemical potential in left reservoir
μ_2	Electrochemical potential in right reservoir
$v_x^+(\mathbf{k})$	Velocity of electrons in k-space
$f(\mu_1)$	Fermi function at electrochemical potential μ_1
π	Ratio of the circumference of circle to its diameter
e	Electron charge
$\sum_{\mathbf{k}'} T^{++}(\mathbf{k},\mathbf{k}')$	Probability that electrons with wave vector **k** will be transmitted
$\mathbf{k}$	Electron **w**ave vector
I	Electric current
A	Area
V	Electric bias or voltage difference
G	Landauer conductance
E_F	Fermi energy
h	Planck's constant
$\hbar$	$h/2\pi$
m	Mass of electron
∇	Gradient operator
E	Energy of the electron
r	Reflection amplitude

t	Transmission amplitude
T	Transmission probability
$\mathbf{j}$	Current density
ρ	Electron density
R	Reflection probability
$\phi_{i\alpha}$	Atomic orbitals centered at site, i
α	Label to distinguish different orbitals centered on the same site
i	Atomic site label
$C_{i\alpha}$	Wave function coefficient for orbital, $\phi_{i\alpha}$
LCAO	Linear Combination of Atomic Orbitals
$H_{i\alpha,j\beta}$	Hamiltonian matrix elements
E_A	Onsite energy for A atom
E_B	Onsite energy for B atom
E_C	Onsite energy for C atom
ε	Dimensionless parameter E/w
ε_A	Dimensionless parameter E_A/w
ε_B	Dimensionless parameter E_B/w
ε_C	Dimensionless parameter E_C/w
w	Hopping matrix element

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CHAPTER 1: INTRODUCTION

The earliest concept critical to understanding quantum tunneling was introduced by Louis de Broglie. De Broglie proposed in 1923 that waves of matter have a wavelength inversely proportional to their momentum. In 1927, Friedrich Hund was the first to make use of the concept of quantum mechanical barrier penetration [1]. Quantum tunneling of electrons cannot be directly perceived other than on the quantum mechanical scale. Classical mechanics cannot explain tunneling phenomena. Quantum mechanical tunneling happens when particles move through a barrier that is deemed impenetrable by classical mechanical standards. This barrier can be a region of high energy, a vacuum, or an insulator.

Tunneling plays an essential role in several physical, chemical, and biological phenomena. In field emission, an electron can jump from the surface of a metal into a vacuum by tunneling through a potential barrier. The electron is allowed to tunnel through the vacuum if the electric field is large enough and the barrier is thin enough. This is called cold emission. Semiconductors are another example where tunneling can occur. Electron tunneling through an insulating barrier is important for flash devices. Tunneling can also be seen in radioactive decay. In the world of nanotechnology, quantum tunneling can be seen in scanning tunneling microscopes, transistors, and even touch screens.

Consider a particle with energy E in the inner region of a one-dimensional potential well of height V. Assume that the walls of the well have thickness, t. According to classical mechanics, if E is less than V, the particle will remain in the well forever. If E is greater than V, then the particle will escape the potential well. This is not the case, according to quantum mechanics. Even if V is greater than E, there is a possibility that the particle will tunnel through the barrier. The particle can escape even if its energy is less than V, but the probability depends on the difference between E and V and on the thickness of the walls surrounding the well.

For tunneling of electrons in solids, the potential well is typically a metallic region where electrons at the Fermi energy can propagate and the barrier is generally a material in which electrons at the Fermi energy cannot propagate, in other words there is typically a gap at the Fermi energy for the barrier material. Even though electrons cannot propagate indefinitely, there will be an evanescent state that extends from the metal into the tunneling barrier. These evanescent states play a central role in tunneling. The evanescent states arise from the complex band structure of the insulator which determines how they decay in the insulator. [2,3]

The electron tunneling phenomenon arises from the wave nature of the electrons and results from the fact that when a wave encounters an interface, it may be partially reflected and partially transmitted. This interfacial reflectance will lead to an interfacial or junction resistance. In this thesis, we shall treat tunneling similar to a scattering problem in which an incident wave on a barrier is partially transmitted and partially reflected. The transmission probability will be related to the conductance using a model due to Landauer.[4] Brinkman, Dynes, and Rowell treat tunneling in this way using a simple barrier model, but their model treats the electron dispersion using the free electron model. In this approach it is not possible to investigate tunneling in the gap between a valence band and a conduction band. We shall remedy this limitation by using the tight-binding model to generate a barrier with a gap separating a valence band and a conduction band. [5]

In an alternative model for tunneling used by Bardeen [6] and Slonczewski [2], one begins with two electrodes separated by an insulator so thick that no tunneling occurs. Then the two electrodes are regarded as completely independent systems. When they are brought closer together so that their wave functions begin to overlap, tunneling occurs. The overlap matrix elements correspond directly to the hopping integrals of the tight-binding method. Perturbation theory is used to calculate the tunneling probability from the matrix elements. It is assumed that the states between which tunneling takes place are those of the electrodes unperturbed by the tunneling process (electrodes separated by an infinitely thick insulator).

CHAPTER 2: TUNNELING

CHAPTER 2.1: LANDAUER CONDUCTANCE FORMULA

Ballistic transport, including tunneling of electrons, was treated by Landauer in 1970. [4] In this approach, one imagines two electron reservoirs separated by leads and a sample (in our case, a tunnel barrier) as shown in Figure 1.

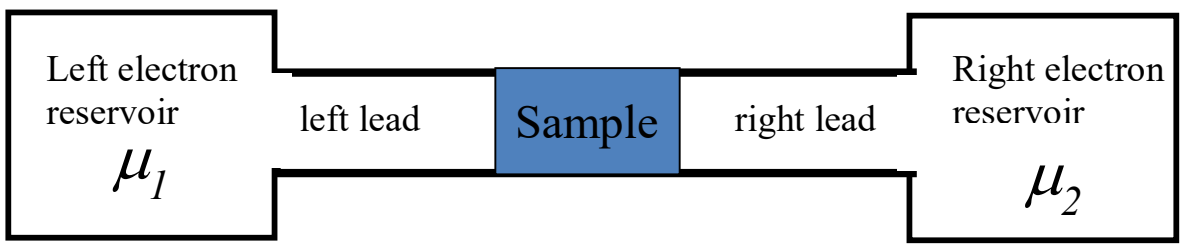

Figure 1. Geometry for derivation of Landauer transport formula showing left and right electron reservoirs separated by leads and a sample.

Within each reservoir we consider the electrons to be (locally) in equilibrium at chemical potentials μ_1 on the left and μ_2 on the right. We also imagine that there are conduction channels that connect the reservoirs. These channels consist of the transverse modes of the leads. In particular, for a system with two dimensional periodicity perpendicular to the leads, they will consist of the values of the crystal momentum of the two dimensional Brillouin zone. The number of these transverse modes is proportional to the cross sectional area of the leads. The reservoirs are viewed as emitters of electrons, the one on the left emitting right-going electrons and the one on the right emitting left-going electrons, very much like the classical black body emitting radiation.

The Landauer formalism relates the net current through the sample between the two reservoirs to the emitted currents. The right-going current from the left reservoir, for example, will be given by integrating over all of the states in the left reservoir. Only the right going states ($v_x^+(\mathbf{k})$) will contribute

to this current. The occupation of the states is given by the Fermi function, ($f(\mu_1)$) so that in the absence of scattering the right-going current density in the leads in our semi-classical approximation for a single spin channel would be

$$J^+ = \frac{e}{(2\pi)^3} \int d^3k \; v_x^+(\mathbf{k}) f(\mu_1) \tag{1}$$

where x is the direction from left to right leading from one reservoir to the other, $f(\mu_1)$ is the electron distribution function, $v_x^+(\mathbf{k})$ is the electron velocity in the z-direction, and e is the electron charge. If scattering (*i.e.* anything that breaks the 3-dimensional periodicity of the leads) is present, the forward scattered electrons will still get through and contribute to the right-going current,

$$J^+ = \frac{e}{(2\pi)^3} \int d^3k \; v_x^+(\mathbf{k}) f(\mu_1) \sum_{\mathbf{k}'} T^{++}(\mathbf{k},\mathbf{k}'), \tag{2}$$

where $\sum_{\mathbf{k}'} T^{++}(\mathbf{k},\mathbf{k}')$ is the probability that electrons with momentum **k** will be transmitted, i.e. have a positive component of velocity in the x -direction after scattering. Let the component of the momentum, $\mathbf{k}$, parallel to the interface be $\mathbf{k}_{\parallel}$ and the component perpendicular to the interface be k_x . It can be shown that $v_x^+(\mathbf{k})$ is related to the energy dispersion by,

$$v_x^+(\mathbf{k}) = \frac{1}{\hbar} \frac{\partial E(\mathbf{k})}{\partial k_x} . \tag{3}$$

Usually there will be more than one band so there should be an index, e.g. n, that should be summed over to obtain the current density, however, for simplicity, we will assume that $\mathbf{k}$ includes the band index and the integral over $\mathbf{k}$ includes a sum over bands which is not shown explicitly.

If we separate the integral over momentum into integrals over $\mathbf{k}_{\|}$ and k_x, we can write J^+ as

$$J^+ = \frac{e}{(2\pi)^2}\int d^2k_{\|}\frac{1}{2\pi}\int dk_x \ \frac{1}{\hbar}\frac{\partial E(\mathbf{k})}{\partial k_x} f(\mu_1)\sum_{\mathbf{k}'} T^{++}(\mathbf{k},\mathbf{k}'), \tag{4}$$

or,

$$J^+ = \frac{e}{A}\sum_{\mathbf{k}_{\|}}\frac{1}{2\pi}\int dk_x \ \frac{1}{\hbar}\frac{\partial E(\mathbf{k})}{\partial k_x} f(\mu_1)\sum_{\mathbf{k}'} T^{++}(\mathbf{k},\mathbf{k}'), \tag{5}$$

where we have used a standard expression to relate the integral over the two dimensional Brillouin zone to a sum. Finally, we convert the integral over k_x into an integral over energy and use the expression *I=JA* to obtain,

$$I^+ = \frac{e}{h}\int^{\mu_1} dE \ \sum_{\mathbf{k}_{\|},\mathbf{k}_{\|}'} T^{++}(\mathbf{k}_{\|},\mathbf{k}_{\|}'). \tag{6}$$

Similarly, we can obtain the current in the $-x$ direction,

$$I^{-} = \frac{e}{h}\int^{\mu_2} dE \sum_{\mathbf{k}_{\parallel},\mathbf{k}_{\parallel}^{'}} T^{--}(\mathbf{k}_{\parallel},\mathbf{k}_{\parallel}^{'}). \tag{7}$$

Time reversal invariance of the Schrödinger equation allows us to equate the transmission probability left to right to the transmission probability right to left, $T^{++} = T^{--}$. If $\mu_1 = \mu_2$ the current from electrons whose origin is on the left cancels that of the electrons originating on the right so that the net current would be zero.

If we apply a small positive bias voltage V so that $\mu_1 - \mu_2 = eV$, then the net current will come from the energy "window" between μ_1 and μ_2, and the net current (right-going minus left-going) can be written as

$$\begin{aligned} I = \; I^{+} - I^{-} &= \frac{e}{h}\int^{\mu_1} dE \sum_{\mathbf{k}_{\parallel},\mathbf{k}_{\parallel}^{'}} T^{++}(\mathbf{k}_{\parallel},\mathbf{k}_{\parallel}^{'}) - \frac{e}{h}\int^{\mu_2} dE \sum_{\mathbf{k}_{\parallel},\mathbf{k}_{\parallel}^{'}} T^{--}(\mathbf{k}_{\parallel},\mathbf{k}_{\parallel}^{'}) \\ &= \frac{e}{h}\left(\mu_1 - \mu_2\right) \sum_{\mathbf{k}_{\parallel},\mathbf{k}_{\parallel}^{'}} T^{++}(\mathbf{k}_{\parallel},\mathbf{k}_{\parallel}^{'}) \\ &= \frac{e^2}{h} \sum_{\mathbf{k}_{\parallel},\mathbf{k}_{\parallel}^{'}} T^{++}(\mathbf{k}_{\parallel},\mathbf{k}_{\parallel}^{'}) \frac{\mu_1 - \mu_2}{e}. \end{aligned} \tag{8}$$

Using the definition of the bias voltage, $V = \frac{\mu_1 - \mu_2}{e}$, and the definition of conductance, $G = IV$, the net current yields the Landauer conductance formula (for a single spin channel),

$$G = \frac{I}{V} = \frac{e^2}{h} \sum_{\mathbf{k}_{\parallel},\mathbf{k}_{\parallel}^{'}} \left[T^{++}(\mathbf{k}_{\parallel},\mathbf{k}_{\parallel}^{'}) \right]_{E_F} . \qquad (9)$$

CHAPTER 2.2: SIMPLE BARRIER MODEL FOR TUNNELING

As an example, the Landauer formula can be used to calculate the conductance for a simple model in which the leads are described by free electrons and the sample is modeled as a potential step or barrier. This allows us to reduce the problem of calculating the transmission probability to a one dimensional problem that can be solved by requiring continuity of the wave function and its derivative at the boundaries between the sample and the leads. We begin with the Schrödinger equation, in the general representation in which the Hamiltonian and wave function depend on both time and position,

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V\left(\vec{r},t\right)\right)\Phi\left(\vec{r},t\right) = i\hbar\frac{\partial}{\partial t}\Phi\left(\vec{r},t\right). \tag{10}$$

Here m is the mass of the electron, and $\hbar$ is Planck's constant. In our case, the potential, $V\left(\vec{r}\right)$, and the Hamiltonian,

$$H = -\frac{\hbar^2}{2m}\nabla^2 + V\left(\vec{r}\right), \tag{11}$$

are independent of time, so the solution to the Schrödinger equation can be separated into time and position dependences by writing the wave function as the product of space and time dependent functions, $\Phi\left(\vec{r},t\right) = \Psi\left(\vec{r}\right) f\left(t\right)$ so that the Schrödinger equation becomes,

$$-\frac{\hbar^2}{2m} f(t)\nabla^2\Psi(\vec{r}) + V(\vec{r})\Psi(\vec{r}) f(t) = i\hbar\Psi(\vec{r})\frac{\partial}{\partial t} f(t). \tag{12}$$

We divide by $\Psi(\vec{r}) f(t)$ to obtain,

$$-\frac{\hbar^2}{2m}\frac{1}{\Psi(\vec{r})}\nabla^2\Psi(\vec{r}) + V(\vec{r}) = i\hbar\frac{1}{f(t)}\frac{\partial}{\partial t} f(t), \tag{13}$$

and we choose a separation constant, E, the electron energy, to separate the Schrödinger equation into two equations:

$$-\frac{\hbar^2}{2m}\frac{1}{\Psi(\vec{r})}\nabla^2\Psi(\vec{r}) + V(\vec{r}) = E \tag{14}$$

and

$$i\hbar\frac{1}{f(t)}\frac{\partial}{\partial t} f(t) = E. \tag{15}$$

Eq. (15) can be integrated to yield,

$$f(t) = e^{-i\frac{E}{\hbar}t}. \tag{16}$$

The wave function becomes

$$\Phi(\vec{r},t)=\Psi(\vec{r})e^{-i\frac{E}{\hbar}t} \tag{17}$$

where $\Psi(\vec{r})$ depends on $V(\vec{r})$ and is found by solving the time independent Schrödinger equation,

$$\left(-\frac{\hbar^2}{2m}\nabla^2+V(\vec{r})\right)\Psi(\vec{r})=E\Psi(\vec{r}), \tag{18}$$

with boundary conditions appropriate to incoming electrons from $x=-\infty$ and transmitted electrons for $x=+\infty$. $V(\vec{r})=V(x)$ is the potential which is assumed to be zero except in the region occupied by the sample or tunnel barrier which extends from $x=0$ to $x=d$, where it is a constant, V.

Because $V(\vec{r})=V(x)$ is only a function of x, we can separate variables by assuming a wave function of the form,

$$\Psi(\vec{r})=\Psi(x,y,z)=\psi(x)\phi(y)\zeta(z). \tag{19}$$

We substitute this form for $\Psi(\vec{r})$ into the Schrödinger equation to obtain

$$\begin{aligned}-\frac{\hbar^2}{2m}&\left[\phi(y)\zeta(z)\frac{\partial^2\psi(x)}{\partial x^2}+\psi(x)\zeta(z)\frac{\partial^2\phi(y)}{\partial y^2}+\psi(x)\phi(y)\frac{\partial^2\zeta(z)}{\partial z^2}\right]\\&+V(x)\psi(x)\phi(y)\zeta(z)=E\psi(x)\phi(y)\zeta(z).\end{aligned} \tag{20}$$

Dividing Equation (20) by Equation (19) yields,

$$\frac{1}{\psi(x)}\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x)+V(x)\psi(x)\right]+\frac{1}{\phi(y)}\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial y^2}\phi(y)\right]$$
$$+\frac{1}{\zeta(z)}\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2}\zeta(z)\right]=E. \tag{21}$$

Each of the three terms on the left side of the equals sign depends on only one of the x, y or z coordinates. Hence we have three independent equations:

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x)+V(x)\psi(x)=E_1\psi(x) \tag{22}$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial y^2}\phi(y)=E_2\phi(y) \tag{23}$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2}\zeta(z)=E_3\zeta(z) \tag{24}$$

where

$$E_1+E_2+E_3=E\,. \tag{25}$$

Equations (23) and (24) have plane wave solutions,

$$\phi(y)=\exp(ik_y y), \tag{26}$$

$$\zeta(z)=\exp(ik_z z), \tag{27}$$

with

$$\frac{\hbar^2 k_y^2}{2m} = E_2 \tag{28}$$

and

$$\frac{\hbar^2 k_z^2}{2m} = E_3 \,. \tag{29}$$

Thus

$$E_1 = E - \frac{\hbar^2}{2m}\left(k_y^2 + k_z^2\right) = E - \frac{\hbar^2}{2m} k_{\parallel}^2 \tag{30}$$

and Equation (22) may be written as,

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi\left(x\right) = \left(E - \frac{\hbar^2}{2m} k_{\parallel}^2 - V\left(x\right)\right)\psi\left(x\right), \tag{31}$$

which may be written in regions 1 and 3 where $V\left(x\right) = 0$ as

$$\frac{\partial^2 \psi\left(x\right)}{\partial x^2} = -k^2 \psi\left(x\right) \tag{32}$$

with

$$k^2 = \frac{2mE}{\hbar^2} - k_{\parallel}^2 , \tag{33}$$

and in region 2, where $V(x) = V$ as

$$\frac{\partial^2 \psi(x)}{\partial x^2} = -k'^2 \psi(x) \tag{34}$$

where

$$k'^2 = \frac{2m}{\hbar^2}(E - V) - k_{\parallel}^2 . \tag{35}$$

In fact, we shall be interested in the energy range for which k'^2 is negative.

When the energy of the electron, E, is lower than the barrier potential V, the wave functions may be written for regions, 1, 2 and 3 as:

$$\psi_1 = e^{ikx} + re^{-ikx}, \quad k = \sqrt{\frac{2mE}{\hbar^2} - k_{\parallel}^2} \quad \text{(region 1)} \tag{36}$$

$$\psi_2 = Ae^{k'x} + Be^{-k'x}, \quad k' = \sqrt{\frac{2m(V-E)}{\hbar^2} + k_{\parallel}^2} \quad \text{(region 2)} \tag{37}$$

$$\psi_3 = te^{ik''x}, \quad k'' = \sqrt{\frac{2mE}{\hbar^2} - k_{\parallel}^2} = k \quad \left(\text{region 3}\right) \tag{38}$$

Equation (36) represents the boundary condition that in region 1, the wave function consists of an incident plane wave traveling in the $+x$ direction and a reflected wave of relative amplitude r traveling in the $-x$ direction. Equation (38) represents the boundary condition that in region 3 there is no wave incident from the right, only a transmitted wave of relative amplitude t. The coefficients, $r, t, A,$ and B, are determined from the boundary conditions and the requirements that the wave function and the derivatives should be continuous. If we assume that the left and right leads are made from the same material, then k and k'' are equal and will be represented by k. ψ_1 and ψ_3 are the wave functions for the left (1) and right leads (3) respectively, and ψ_2 is the wave function for the barrier region (2).

Requiring continuity of wave function and derivative at the interfaces yields,

$$\psi_1\big|_{x=0} = \psi_2\big|_{x=0} \qquad \psi_2\big|_{x=a} = \psi_3\big|_{x=d}$$

$$\left.\frac{\partial\psi_1}{\partial x}\right|_{x=0} = \left.\frac{\partial\psi_2}{\partial x}\right|_{x=0} \qquad \left.\frac{\partial\psi_2}{\partial x}\right|_{x=a} = \left.\frac{\partial\psi_3}{\partial x}\right|_{x=d} \tag{39}$$

$$1 + r = A + B \qquad Ae^{k'd} + Be^{-k'a} = te^{ikd}$$

$$1 - r = \left(\frac{k'}{ik}\right)\left(A - B\right) \qquad Ae^{k'd} - Be^{-k'd} = \left(\frac{ik}{k'}\right)te^{ikd} \tag{40}$$

This set of four linear equations can be solved to determine, $A,\ B,\ r$ and t

$$A = \frac{k\left(k + ik'\right)e^{k'd}}{2ikk'\cosh k'd + (k^2 - k'^2)\sinh k'd}, \tag{41}$$

$$B = -\frac{k\left(k - ik'\right)e^{-k'd}}{2ikk'\cosh k'd + (k^2 - k'^2)\sinh k'd}, \tag{42}$$

$$t = \frac{2ikk'}{2ikk'\cosh k'd + (k^2 - k'^2)\sinh k'd}, \tag{43}$$

and

$$r = \frac{(k^2 + k'^2)\sinh k'd}{2ikk'\cosh k'd + (k^2 - k'^2)\sinh k'd}. \tag{44}$$

The transmission and reflection amplitudes are given by r and t, respectively.

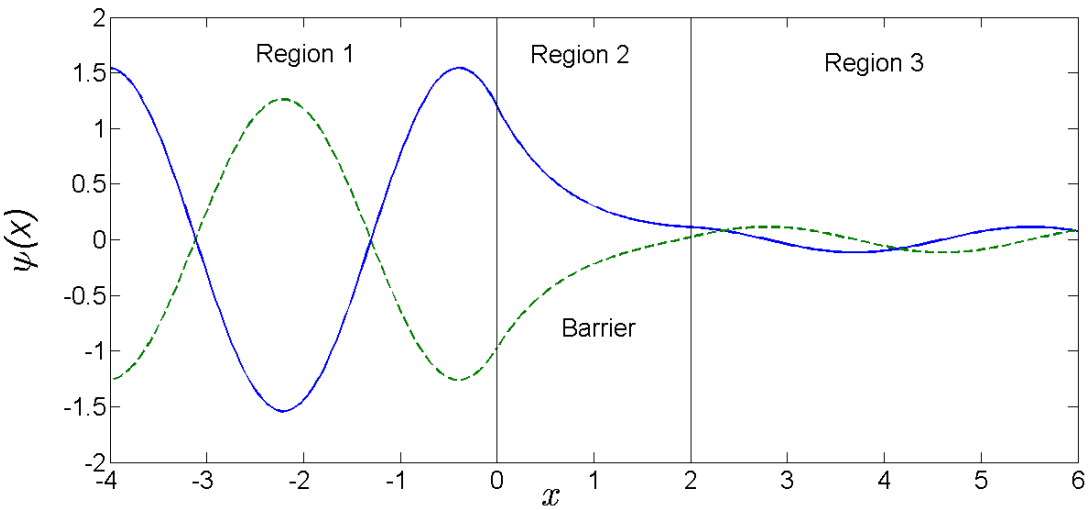

Figure 2: Tunneling wave function for the simple barrier model for a fixed value of $k_{\parallel}$. For this example, the barrier extends from $x = 0$ to $x = 2$.

The transmission and reflection probabilities, for a given value of $\mathbf{k}_{\parallel}$ are given by

$$T = tt^* = \frac{4k^2k'^2}{4k^2k'^2\cosh^2 k'd + \left(k^2 - k'^2\right)^2 \sinh^2 k'd} = \frac{4k^2k'^2}{4k^2k'^2 + \left(k^2 + k'^2\right)^2 \sinh^2 k'd} . \qquad (45)$$

and $R = rr^* = \dfrac{\left(k^2 + k'^2\right)^2 \sinh^2 k'd}{4k^2k'^2 + \left(k^2 + k'^2\right)^2 \sinh^2 k'd}$.

It is important to note that the transmission probability is only given by the simple relation $T = t^*t$ when the leads are the same on the two sides of the barrier. If they are different, one must either compare the transmitted current to the incident current or carefully normalize the incident and transmitted wave

functions so that they carry the same current and flux. We will return to this point again after we discuss the current density.

To obtain the conductance, we must integrate the transmission probability in Equation (37) over $\mathbf{k}_{\parallel}$. If we define

$$k_F^2 = \frac{2mE}{\hbar^2} \tag{46}$$

and

$$\kappa^2 = \frac{2mV}{\hbar^2}, \tag{47}$$

then the transmission probability may be written,

$$T\left(E,V,k_{\parallel}\right) = \frac{4\left(k_F^2 - k_{\parallel}^2\right)\left(\kappa^2 - k_F^2 + k_{\parallel}^2\right)}{4\left(k_F^2 - k_{\parallel}^2\right)\left(\kappa^2 - k_F^2 + k_{\parallel}^2\right) + \kappa^4 \sinh^2\sqrt{\kappa^2 - k_F^2 + k_{\parallel}^2}\, d}, \tag{48}$$

and the (single spin-channel) conductance from the Landauer formula may be written, taking advantage of the conservation of transverse momentum as an integral over $k_{\parallel}$,

$$G = \frac{e^2}{h}\frac{A}{2\pi}\int_0^{k_F} k_{\parallel} dk_{\parallel} T\left(E,\mathrm{V},k_{\parallel}\right). \tag{49}$$

Setting

$$x = \frac{k_F}{\kappa} \tag{50}$$

and

$$z = \frac{k_{\parallel}}{\kappa}\,, \tag{51}$$

this may be written as,

$$G = \frac{e^2}{h}\frac{A}{2\pi}\kappa^2 \int_0^x z dz \frac{4\left(x^2 - z^2\right)\left(1 - x^2 + z^2\right)}{4\left(x^2 - z^2\right)\left(1 - x^2 + z^2\right) + \sinh^2\left(\kappa d\sqrt{1 - x^2 + z^2}\right)}\,. \tag{52}$$

A change of the variable of integration using,

$$u^2 = 1 - x^2 + z^2 \tag{53}$$

yields,

$$G = \frac{e^2}{h}\frac{A}{2\pi}\kappa^2 \int_{\sqrt{1-x^2}}^{1} u du \frac{4u^2\left(1 - u^2\right)}{4u^2\left(1 - u^2\right) + \sinh^2\left(\kappa d u\right)}\,. \tag{54}$$

It should be noted that this result is only valid in the limit of low bias both because we have restricted the potential to be the same in both leads and because we have assumed a constant potential for the barrier region.

In the limit of $d \to 0$ in which the barrier vanishes and the transmission probability becomes unity, Equation (54) can be integrated trivially to give,

$$G = \frac{e^2}{h} \frac{A}{(2\pi)^2} \pi k_F^2 , \tag{55}$$

which is the Sharvin single spin-channel conductance for a contact. [7] The Sharvin conductance can be viewed as $\frac{e^2}{h}$ times the number of conductance channels. The number of conductance channels per unit area is the projection of the Fermi sphere onto a plane perpendicular to the $x-$axis divided by $(2\pi)^2$, which may be viewed as a square wave length per conductance channel.

In the limit of $d \to \infty$, Equation (54) yields,

$$\begin{aligned} G &= \frac{e^2}{h} \frac{A}{2\pi} \frac{\kappa}{2d} 16 \frac{E_F}{V} \left(1 - \frac{E_F}{V}\right)^{\frac{3}{2}} \exp\left(-2\kappa d \sqrt{1 - \frac{E_F}{V}}\right) \\ &= \frac{e^2}{h} \frac{A}{2\pi} \frac{\kappa}{2d} \left(1 - \frac{E_F}{V}\right)^{\frac{1}{2}} T\left(E_F, V, k_{\parallel} = 0\right) \\ &= \frac{e^2}{h} \frac{A}{(2\pi)^2} \pi \overline{k_{\parallel}^2} T\left(E_F, V, k_{\parallel} = 0\right) \end{aligned} \tag{56}$$

where $\overline{k_{\parallel}^2} = \frac{\sqrt{\kappa^2 - k_F^2}}{d}$.

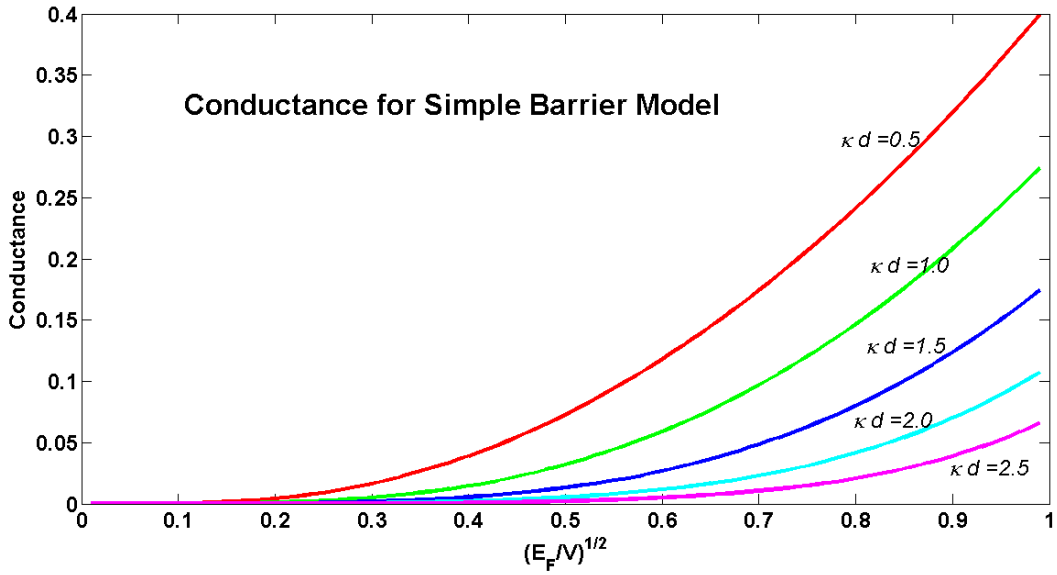

Figure 3: Graph of Conductance as a function of $\sqrt{\frac{E_F}{V}}$ for different values of thickness, *d*. Conductance is expressed in units of $\frac{e^2}{h}\frac{A\kappa^2}{2\pi}$ (see Equation (54)).

CHAPTER 2.3: CURRENT DENSITY

We can think of the probability of finding an electron in a particular spatial region changing due to a probability flow, or current, entering or leaving that region. This definition of the current is chosen so that the probability density will satisfy the continuity equation

$$\nabla \cdot \mathbf{j} = -\frac{\partial \rho}{\partial t}, \tag{57}$$

representing the fact that electrons are conserved. Here, the electron density is represented by

$$\rho(\vec{r},t) = \Phi^*(\vec{r},t)\Phi(\vec{r},t). \tag{58}$$

We can use the time-dependent Schrödinger equation to derive the current. First, we take the time-dependent Schrödinger equation and its complex conjugate:

$$i\hbar \frac{\partial}{\partial t}\Phi(\vec{r},t) = H\Phi(\vec{r},t) = \left[-\frac{\hbar^2}{2m}\nabla^2 + V\right]\Phi(\vec{r},t) \tag{59}$$

and

$$-i\hbar \frac{\partial}{\partial t}\Phi^*(\vec{r},t) = H\Phi^*(\vec{r},t) = \left[-\frac{\hbar^2}{2m}\nabla^2 + V\right]\Phi^*(\vec{r},t). \tag{60}$$

Multiplying the first of these equations by $\Phi^*(\vec{r},t)$ and the second by $\Phi(\vec{r},t)$ yields

$$\Phi^*(\vec{r},t)i\hbar\frac{\partial}{\partial t}\Phi(\vec{r},t)=\Phi^*(\vec{r},t)H\Phi(\vec{r},t)=\Phi^*(\vec{r},t)\left[-\frac{\hbar^2}{2m}\nabla^2+V\right]\Phi(\vec{r},t) \tag{61}$$

and

$$-\Phi(\vec{r},t)i\hbar\frac{\partial}{\partial t}\Phi^*(\vec{r},t)=\Phi(\vec{r},t)H\Phi^*(\vec{r},t)=\Phi(\vec{r},t)\left[-\frac{\hbar^2}{2m}\nabla^2+V\right]\Phi^*(\vec{r},t). \tag{62}$$

Subtracting these two equations yields

$$i\hbar\frac{\partial}{\partial t}\left[\Phi(\vec{r},t)\Phi^*(\vec{r},t)\right]=-\frac{\hbar^2}{2m}\left[\Phi^*(\vec{r},t)\nabla^2\Phi(\vec{r},t)-\Phi(\vec{r},t)\nabla^2\Phi^*(\vec{r},t)\right]. \tag{63}$$

which can be written as

$$\frac{\partial}{\partial t}\rho(\vec{r},t)=-\frac{\hbar}{2mi}\nabla\cdot\left[\Phi^*(\vec{r},t)\nabla\Phi(\vec{r},t)-\Phi(\vec{r},t)\nabla\Phi^*(\vec{r},t)\right]. \tag{64}$$

We can now see that this becomes the continuity equation if we identify,

$$\mathbf{j}=\frac{\hbar}{2mi}\left[\Phi^*(\vec{r},t)\nabla\Phi(\vec{r},t)-\Phi(\vec{r},t)\nabla\Phi^*(\vec{r},t)\right], \tag{65}$$

as the electron current. Since the gradient operator does not operate on the time dependent part of the wave function, this may be written as

$$\mathbf{j} = \frac{\hbar}{2mi}\left[\Psi^*(\vec{r})\nabla\Psi(\vec{r}) - \Psi(\vec{r})\nabla\Psi^*(\vec{r})\right], \tag{66}$$

and the current in the $x-$direction (for a given value of $\mathbf{k}_{\|}$) is given by

$$j_{ix} = \frac{\hbar}{2mi}\left[\psi_i^* \frac{\partial \psi_i}{\partial x} - \psi_i \frac{\partial \psi_i^*}{\partial x}\right], \quad (i = 1-3) \tag{67}$$

where $\psi_i(x, k_{\|})$ is given by Equations (36-38) for the simple barrier model.

For each region (1, 2, and 3), the currents are represented by

$$j_{1x} = \frac{\hbar}{2mi}\left[\psi_1^* \frac{\partial}{\partial x}\psi_1 - \psi_1 \frac{\partial}{\partial x}\psi_1^*\right] = \frac{\hbar k}{m}\left(1 - |r|^2\right) \text{ (region 1)} \tag{68}$$

$$j_{2x} = \frac{\hbar}{2mi}\left[\psi_2^* \frac{\partial}{\partial x}\psi_2 - \psi_2 \frac{\partial}{\partial x}\psi_2^*\right] = \frac{\hbar k'}{mi}\left(B^* A - A^* B\right) \text{ (region 2)} \tag{69}$$

$$j_{3x} = \frac{\hbar}{2mi}\left[\psi_3^* \frac{\partial}{\partial x}\psi_3 - \psi_3 \frac{\partial}{\partial x}\psi_3^*\right] = \frac{\hbar k}{m}\left(|t|^2\right) \text{ (region 3)} \tag{70}$$

The reflection and transmission probabilities in the simple barrier model were found to be,

$$R = |r|^2 = \frac{\left(k^2 + k'^2\right)^2 \sinh^2 k'd}{\left(2k'k\right)^2 + \left(k^2 + k'^2\right)^2 \sinh^2 k'd} \tag{71}$$

and

$$T = |t|^2 = \frac{\left(2k'k\right)^2}{\left(2k'k\right)^2 + \left(k^2 + k'^2\right)^2 \sinh^2 k'd}. \tag{72}$$

In the left lead, we have,

$$\begin{aligned} j_{1x} &= \frac{\hbar}{2mi}\left(\psi_1^* \frac{\partial}{\partial x}\psi_1 - \psi_1 \frac{\partial}{\partial x}\psi_1^*\right) = \frac{\hbar k}{m}\left(1 - |r|^2\right) \\ &= \frac{\hbar k}{m}\left[1 - \frac{\left(k^2 + k'^2\right)^2 \sinh^2 k'd}{\left(2k'k\right)^2 + \left(k^2 + k'^2\right)^2 \sinh^2 k'd}\right] \\ &= \frac{\hbar k}{m}\left[\frac{\left(2k'k\right)^2 + \left(k^2 + k'^2\right)^2 \sinh^2 k'd - \left(k^2 + k'^2\right)^2 \sinh^2 k'd}{\left(2k'k\right)^2 + \left(k^2 + k'^2\right)^2 \sinh^2 k'd}\right] \\ &= \frac{\hbar k}{m}\left[\frac{\left(2k'k\right)^2}{\left(2k'k\right)^2 + \left(k^2 + k'^2\right)^2 \sinh^2 k'd}\right] = v_x\left(k_{\parallel}\right) T\left(k_{\parallel}\right) \end{aligned} \tag{73}$$

,

and in the barrier region, the current is given by,

$$
\begin{aligned}
j_{2x} &= \frac{\hbar}{2mi}\left(\psi_2^*\frac{\partial}{\partial x}\psi_2 - \psi_2\frac{\partial}{\partial x}\psi_2^*\right) = \frac{\hbar k'}{2m}\left(B^*A - A^*B\right) \\
&= \frac{\hbar k'}{mi}\left[\frac{k\left(k+ik'\right)e^{-k'a}}{-2ik'k\cosh k'd + \left(k^2-k'^2\right)\sinh k'd} + \frac{k\left(k+ik'\right)e^{k'a}}{2ik'k\cosh k'd + \left(k^2-k'^2\right)\sinh k'd}\right] \\
&+ \frac{\hbar k'}{mi}\left[\frac{k\left(k-ik'\right)e^{k'a}}{-2ik'k\cosh k'd + \left(k^2-k'^2\right)\sinh k'd} + \frac{k\left(k-ik'\right)e^{-k'a}}{2ik'k\cosh k'd + \left(k^2-k'^2\right)\sinh k'd}\right] \\
&= \frac{\hbar k'}{mi}\left[\frac{k^4 + 2k^3ik' - k'^2k^2 - k^4 + 2k^3ik' + k'^2k^2}{4k'^2k^2\cosh^2 k'd + \left(k^2-k'^2\right)^2\sinh^2 k'd}\right] \\
&= \frac{\hbar k}{m}\left[\frac{\left(2k'k\right)^2}{\left(2k'k\right)^2 + \left(k^2+k'^2\right)^2\sinh^2 k'd}\right] = v_x\left(k_{\parallel}\right)T\left(k_{\parallel}\right).
\end{aligned}
\tag{74}
$$

It is interesting to note that the exponentially increasing as well as the exponentially decreasing component of the wave function in the barrier region must be present, otherwise the current in this region will vanish (see Equation (69)). A semi-infinite barrier will support an exponentially decreasing evanescent wave, but it carries no current.

In the right lead, the current is given by,

$$
\begin{aligned}
j_{3x} &= \frac{\hbar}{2mi}\left(\psi_3^*\frac{\partial}{\partial x}\psi_3 - \psi_3\frac{\partial}{\partial x}\psi_3^*\right) = \frac{\hbar k}{m}\left|t\right|^2 \\
&= \frac{\hbar k}{m}\left[\frac{\left(2k'k\right)^2}{\left(2k'k\right)^2 + \left(k^2+k'^2\right)^2\sinh^2 k'd}\right] = v_x\left(k_{\parallel}\right)T\left(k_{\parallel}\right).
\end{aligned}
\tag{75}
$$

Thus the current is conserved throughout each region of the tunneling process. Second, the identity, $R+T=1$, is satisfied. Last, we should note that as the barrier becomes thicker (d increases) or the barrier gets taller (k' increases), R increases and the conductance and current decreases.

In Equations (72-75) we have identified the transmission probability with the absolute square of the transmission amplitude, $T\left(k_{\parallel}\right)=t^{*}t$. This is only valid if the left and right leads are the same or if the incident and transmitted wave functions are normalized to carry the same current. In the general case with un-normalized incident and transmitted wave functions, $e^{ik_{Left}x}$, and $e^{ik_{Right}x}$, the transmission probability is obtained by taking the ratio of the transmitted current to the incident current, $T\left(k_{\parallel}\right)=v_{Left}\left(k_{\parallel}\right)t^{*}\left(k_{\parallel}\right)t\left(k_{\parallel}\right)/v_{Right}\left(k_{\parallel}\right)$.

CHAPTER 3: TIGHT-BINDING APPROXIMATION

CHAPTER 3.1: LCAO OR TIGHT-BINDING MODEL FOR ELECTRONIC STRUCTURE

The simple barrier model has the advantage of simplicity, but it may miss important physics associated with the existence of atoms in real tunneling systems. One obvious limitation is that real barrier materials have both a conduction band and a valence band – the simple barrier model for a tunneling barrier has only a conduction band. In this section we shall develop the tight-binding formalism for electron transport and quantum mechanical tunneling.

The tight-binding approximation is based on the assumption that the electron wave function can be approximated as a linear combination of atomic orbitals (LCAO),

$$\Psi\left(\vec{r}\right) = \sum_{\substack{atomic \\ site,i}} \sum_{orbitals,\alpha} C_{i\alpha}\phi_{i\alpha}\left(\vec{r} - \vec{R}_i\right), \tag{76}$$

where $\phi_{i\alpha}$ represents an atomic orbital centered at site, i, with label, α, distinguishing different orbitals centered on the same site. The $C_{i\alpha}$ represent coefficients which are to be determined. The time independent Schrodinger equation was given in Equation (18). The Schrödinger equation is $H\Psi\left(\vec{r}\right) = E\Psi\left(\vec{r}\right)$, where, in the presence of atoms, the Hamiltonian can be written as

$$H = -\frac{\hbar^2}{2m}\nabla^2 + \sum_i V_i\left(\vec{r} - \vec{R}_i\right), \tag{77}$$

with $V_i\left(\vec{r}-\vec{R}_i\right)$ representing the effective potential associated with site i. It should be noted that we are assuming a "one electron at a time" or "effective field" approximation such as that given by density functional theory. [8]

By substituting the LCAO approximation for the wave function into the Schrödinger equation and assuming that the atomic orbitals are orthonormal, one can convert the Schrödinger equation into a matrix equation,

$$HC = EC \tag{78}$$

or

$$\sum_{sites\ j}\sum_{orbitals\ \beta}\left[H_{i\alpha,j\beta}-E\right]C_{j\beta}=0 \quad \left(\text{all } i \text{ and } \alpha\right) \tag{79}$$

where the Hamiltonian matrix element is given by

$$H_{i\alpha,j\beta}=\left\langle\phi_{i\alpha}\left|H\right|\phi_{j\beta}\right\rangle=\left\langle i\alpha\left|H\right|j\beta\right\rangle=\int d\vec{r}\,\phi_\alpha^*\left(\vec{r}-\vec{R}_i\right)H\phi_\beta\left(\vec{r}-\vec{R}_j\right). \tag{80}$$

Although the assumption that the wave functions are orthonormal is not very realistic, it can be justified by invoking Wannier functions which are local functions obtained by a transformation of the actual energy bands of the material. The Wannier function basis is orthonormal and the Hamiltonian built from a Wannier function basis can often be made to have a relatively short range. [9]

The development of realistic short-ranged tight-binding Hamiltonians is an active area of research. In this thesis we shall employ empirical models based on tight-binding. The empirical tight-binding method develops approximations only for the Hamiltonian matrix elements $H_{i\alpha,j\beta}$ themselves without attempting to model the potential and the explicit form of the LCAO basis functions. The tight-binding models used in this thesis are too simplistic to accurately represent the electronic structure of a solid, but our objective will be to illustrate important physical principles within models that can be solved exactly.

The simplest tight-binding model for an infinite solid would be a one-dimensional chain of one-orbital atoms with only nearest neighbor interaction. The Hamiltonian for such a system would be an infinite tridiagonal matrix with the orbital energy, E_0, on the diagonal and the "hopping matrix element",

$$w = \langle \phi_i \mid H \mid \phi_{i+1} \rangle, \tag{81}$$

above and below the diagonal. In practice, E_0, and w are parameters that would be adjusted to mimic as well as possible the relevant energy band of the solid. The Schrödinger equation will consist of an infinite set of equations,

$$C_i E_0 + wC_{i+1} + wC_{i-1} = EC_i . \tag{82}$$

The infinite set of equations can be solved by use of Bloch's theorem which states that the wave functions on adjacent sites are related by a phase factor, i.e.,

$$C_{i+1} = e^{i\theta} C_i . \tag{83}$$

This ansatz leads to the dispersion relation,

$$E(\theta) = E_0 + 2w\cos\theta. \tag{84}$$

The phase angle in Equation (83) can be either positive or negative. From Equation (84), it is clear that $\pm\theta$ yield the same energy. The positive sign corresponds to a wave propagating in the $+x$ direction. The negative sign corresponds to a wave of the same energy propagating in the opposite direction.

CHAPTER 3.2: TRANSMISSION THROUGH AN INTERFACE IN TIGHT-BINDING

The simplest system that illustrates tunneling in tight-binding has two types of atoms, type-A and type-B atoms, *i.e.* an A-B system. In this model, a semi-infinite chain of A atoms on the left connects to a semi-infinite chain of B atoms on the right. The parameters are chosen such that the A atoms are metallic having a propagating state at the energy, designated by us as the Fermi energy while the parameters for the Hamiltonian describing the chain of B atoms will be chosen so that it will be either an insulator or a metal at this energy. For simplicity we assume a single *s*-symmetry orbital on each A or B site. We will also assume that the electrons are incident from the left, propagating in the chain of A atoms. The parameter *w* represents the matrix element connecting orbitals on adjacent sites. For simplicity, we assume that *w* is the same for the A and B chains and for the matrix element that connects them. E_A and E_B are respectively the on-site energies for the orbitals on sites A and B.

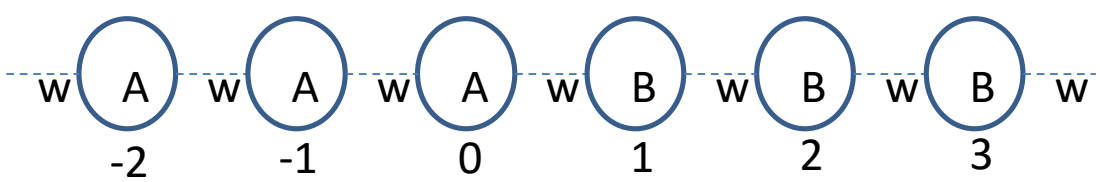

Figure 4: Single *s*-orbital model with semi-infinite chains of A and B atoms. The A atoms extend from $n=-\infty$ to $n=0$. The B atoms extend from $n=1$ to $n=\infty$.

For the left part of the A-B system the wave function ($n \le 0$) is represented by

$$\psi_{Left} = \sum_{-\infty}^{0} c_n^A \phi_n^A \left(r - R_n \right), \tag{85}$$

and for the right part ($n \ge 1$) by,

$$\psi_{Right} = \sum_{n=1}^{\infty} c_n^B \phi_n^B \left(r - R_n \right). \tag{86}$$

The matrix Schrödinger equation (Equation 79) will be an infinite set of equations which includes a semi-infinite set for the left, a semi-infinite set for the right and two equations for the interface,

$$\left(E - E_A \right) c_n^A - w\left(c_{n-1}^A + c_{n+1}^A \right) = 0 \quad (\text{for } n < 0), \tag{87}$$

$$\left(E - E_A \right) c_0^A - w\left(c_{-1}^A + c_1^B \right) = 0 \qquad (\text{for } n = 0), \tag{88}$$

$$\left(E - E_B \right) c_1^B - w\left(c_0^A + c_2^B \right) = 0 \qquad (\text{for } n = 1), \tag{89}$$

and

$$\left(E - E_B \right) c_n^B - w\left(c_{n-1}^B + c_{n+1}^B \right) = 0 \quad (\text{for } n > 1). \tag{90}$$

If we divide these four equations by w, and define

$$E / w = \varepsilon, \tag{91}$$

$$E_A / w = \varepsilon_A, \tag{92}$$

and

$$E_B / w = \varepsilon_B \,, \tag{93}$$

the system becomes,

$$(\varepsilon - \varepsilon_A)\mathrm{c}_n^A - (c_{n-1}^A + c_{n+1}^A) = 0 \quad \text{for } n < 0 \,, \tag{94}$$

$$(\varepsilon - \varepsilon_A)\mathrm{c}_0^A - (c_{-1}^A + c_1^B) = 0 \qquad \text{for } n = 0 \,, \tag{95}$$

$$(\varepsilon - \varepsilon_B)\mathrm{c}_1^B - (c_0^A + c_2^B) = 0 \qquad \text{for } n = 1 \,, \tag{96}$$

and

$$(\varepsilon - \varepsilon_B)\mathrm{c}_n^B - (c_{n-1}^B + c_{n+1}^B) = 0 \quad \text{for } n > 1 \,. \tag{97}$$

The boundary conditions are such that there are incident and reflected wave functions for $n \le 0$, and a transmitted wave function for $n \ge 1$. These can be written as,

$$c_n^A = e^{in\theta_A} + re^{-in\theta_A} \quad (n \le 0) \tag{98}$$

and

$$c_n^B = te^{in\theta_B} \quad (n \ge 0) \,. \tag{99}$$

Substituting the boundary conditions into Equation (95) for $n = 0$ gives,

$$(\varepsilon-\varepsilon_A)(1+r)-(e^{-i\theta_A}+re^{i\theta_A}+te^{i\theta_B})=0\,. \tag{100}$$

Similarly, substituting the boundary conditions into Equation (96) for $n=1$ gives

$$(\varepsilon-\varepsilon_B)te^{i\theta_B}-(te^{2i\theta_B}+1+r)=0\,. \tag{101}$$

The dispersion relations for the left and right sides relate the energy to the phase factors,

$$\varepsilon-\varepsilon_A=e^{-i\theta_A}+e^{i\theta_A} \tag{102}$$

$$\varepsilon-\varepsilon_B=e^{-i\theta_B}+e^{i\theta_B} \tag{103}$$

These can be used to write equations (99) and (100) in terms of *r*, *t* and the phase factors:

$$e^{-i\theta_A}r-te^{i\theta_B}=-e^{i\theta_A} \tag{104}$$

$$-r+t=1. \tag{105}$$

The transmission amplitude can be determined from adding $e^{i\theta_A}$ times the first of these equations to the second,

$$t=\frac{2i\sin\theta_A}{1-e^{-i\theta_B}e^{-i\theta_A}}e^{i\theta_B}\,, \tag{106}$$

and the reflection amplitude from Equation (105),

$$r = \frac{e^{2i\theta_A} - e^{i\theta_A} e^{i\theta_B}}{e^{i\theta_A} e^{i\theta_B} - 1}. \qquad (107)$$

In this case, the reflection probability, $R = rr^* = 1$ if $e^{-i\theta_B} \to z_{real}$. This will happen when the energy is outside the range $-2w < E - E_B < 2w$, since in this case, $\cos\theta_B = \left(E - E_B\right)/2w$ will only have a solution if θ_B is imaginary. We assume $-2w < E - E_A < 2w$, otherwise there would not be an incoming wave.

$$r * r = \left(\frac{e^{i\theta_B} e^{-i\theta_A} - 1}{e^{i\theta_B} e^{i\theta_A} - 1}\right)\left(\frac{e^{-i\theta_B} e^{i\theta_A} - 1}{e^{-i\theta_B} e^{-i\theta_A} - 1}\right) = \frac{1 - \cos(\theta_B - \theta_A)}{1 - \cos(\theta_B + \theta_A)} \qquad when\ z = e^{i\theta_B}.$$

$$r * r = \left(\frac{z_{real} e^{-i\theta_A} - 1}{z_{real} e^{i\theta_A} - 1}\right)\left(\frac{z_{real} e^{i\theta_A} - 1}{z_{real} e^{-i\theta_A} - 1}\right) = 1 \qquad when\ z\ is\ real. \qquad (108)$$

This implies that the reflection probability is unity even though there is a decaying wave of amplitude $c_n = tz^n$ (where $z < 1$) in the semi-infinite chain on the right hand side ($n \geq 1$). We defer a calculation of the transmission probability until after we have derived an expression for the current density in the tight-binding approximation. At that time, we will see that for the case of a semi-infinite chain of B atoms, for energies that do not admit electron propagation, (*i.e.* $e^{-i\theta_B} \to z_{real}$), the current in the B chain vanishes and the transmission probability also vanishes even though there is an exponentially decaying evanescent wave in the B chain.

CHAPTER 3.3: TUNNELING THROUGH A BARRIER IN TIGHT-BINDING

We now consider transmission through a barrier in the tight-binding picture. Our model consists of a semi-infinite chain of A atoms on the left and a semi-infinite chain of A atoms on the right. In between is a finite chain of B atoms.

A-B-A System

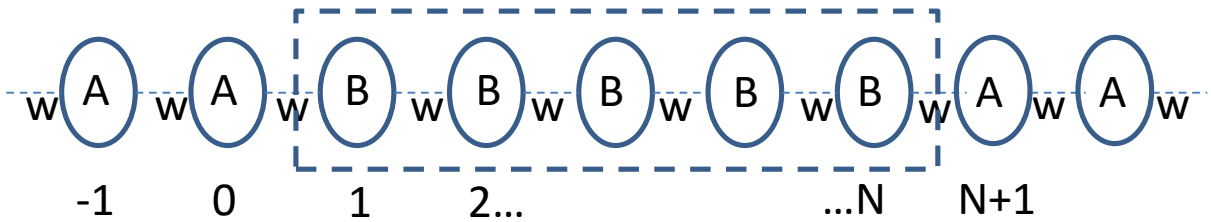

Figure 5: A tunneling system consisting of two semi-infinite chains of A atoms separated by N B atoms. By proper choice of parameters, we can make the A atoms conducting and the B atoms insulating.

The wave functions on the left, middle and right are, as before expressed as a linear combination of atomic orbitals centered on the sites,

$$\psi_{Left} = \sum_{n=-\infty}^{0} c_n^A \phi_n^A \left(r - R_n \right), \tag{109}$$

$$\psi_{Middle} = \sum_{n=1}^{N} c_n^B \phi_n^B \left(r - R_n \right), \tag{110}$$

$$\psi_{Right} = \sum_{n=N+1\infty}^{\infty} c_n^A \phi_n^A \left(r - R_n \right). \tag{111}$$

Using the numbering system shown in Figure 5, we have the two equations that relate the coefficients for the A-chain on the left to the coefficients for the B chain in the center:

$$wc_{-1} + E_A c_0 + wc_1 = Ec_0 \tag{112}$$

and

$$wc_0 + E_B c_1 + wc_2 = Ec_1 . \tag{113}$$

The two equations that relate the coefficients for the wave function in the center to those for the wave function describing the chain on the right:

$$wc_{N-1} + E_B c_N + wc_{N+1} = Ec_N \tag{114}$$

and

$$wc_N + E_A c_{N+1} + wc_{N+2} = Ec_{N+1} . \tag{115}$$

As before, the boundary conditions on the left represent an incoming wave and a reflected wave,

$$c_n = e^{in\theta_A} + re^{-in\theta_A} \ \left(\text{for } n \le 0 \right). \tag{116}$$

In the middle region, the coefficients consist of exponentially increasing and decreasing terms if the energy is outside the region for which the B chain allows propagating solutions. If there are propagating solutions, the exponential functions would be replaced with circular functions representing

left- and right- going waves. Here we will assume for definiteness that the energy is outside the range of the propagating solutions,

$$c_n = Ae^{n\theta_B} + Be^{-n\theta_B} \quad \left(\text{for } 1 \le n \le N\right). \tag{117}$$

On the right side, the boundary condition is that of a transmitted wave propagating in the $+x$ direction,

$$c_n = te^{in\theta_A} \quad (\text{for } n \ge N+1). \tag{118}$$

Substitution of Equation (116) and (117) into the boundary conditions of Equations (112) and (113), the two equations for the left interface yields:

$$\left(e^{-i\theta} + re^{i\theta}\right) + \left(Ae^{\theta_B} + Be^{-\theta_B}\right) = \left(\varepsilon - \varepsilon_A\right)\left(1 + r\right) \tag{119}$$

$$\left(1 + r\right) + \left(Ae^{2\theta_B} + Be^{-2\theta_B}\right) = \left(\varepsilon - \varepsilon_B\right)\left(Ae^{\theta_B} + Be^{-\theta_B}\right). \tag{120}$$

While substitutions of Equations (117) and (118) into the boundary conditions of Equations (113) and (114), the two equations for the right interface yields,

$$\left(Ae^{(N-1)\theta_B} + Be^{-(N-1)\theta_B}\right) + te^{i(N+1)\theta} = \left(\varepsilon - \varepsilon_B\right)\left(Ae^{N\theta_B} + Be^{-N\theta_B}\right) \tag{121}$$

$$\left(Ae^{N\theta_B} + Be^{-N\theta_B}\right) + te^{i(N+2)\theta} = \left(\varepsilon - \varepsilon_A\right)te^{i(N+1)\theta} \tag{122}$$

Using the dispersion relation for A, $\varepsilon = \varepsilon_A + 2\cos\theta_A$, and for B, $\varepsilon = \varepsilon_B + 2\cosh\theta_B$, on the equations for the left interface yields,

$$-re^{-i\theta_A} + \left(Ae^{\theta_B} + Be^{-\theta_B}\right) = e^{i\theta_A} \tag{123}$$

and

$$-r + A + B = 1. \tag{124}$$

Similarly, for the right interface,

$$Ae^{(N+1)\theta_B} + Be^{-(N+1)\theta_B} - te^{i(N+1)\theta_A} = 0 \tag{125}$$

$$Ae^{N\theta_B} + Be^{-N\theta_B} - te^{iN\theta_A} = 0\,. \tag{126}$$

The reflection amplitude, r, can be easily eliminated from Equations (123) and (124) that describe the left interface,

$$A\left(e^{\theta_B} - e^{-i\theta_A}\right) + B\left(e^{-\theta_B} - e^{-i\theta_A}\right) = e^{i\theta_A} - e^{-i\theta_A}\,. \tag{127}$$

Similarly, t, can be eliminated from Equations (125) and (126) that describe the right interface,

$$Ae^{N\theta_B}\left(e^{\theta_B} - e^{i\theta_A}\right) + Be^{-N\theta_B}\left(e^{-\theta_B} - e^{i\theta_A}\right) = 0\,. \tag{128}$$

Equation (128) allows us to obtain A in terms of B.

$$A = -Be^{-2N\theta_B}\frac{\left(e^{-\theta_B} - e^{i\theta_A}\right)}{\left(e^{\theta_B} - e^{i\theta_A}\right)}\,. \tag{129}$$

Then the inhomogeneous equation involving A and B can be solved:

$$B=\frac{\left(e^{i\theta_A}-e^{-i\theta_A}\right)\left(e^{\theta_B}-e^{i\theta_A}\right)}{\left(e^{-\theta_B}-e^{-i\theta_A}\right)\left(e^{\theta_B}-e^{i\theta_A}\right)-e^{-2N\theta_B}\left(e^{-\theta_B}-e^{i\theta_A}\right)\left(e^{\theta_B}-e^{-i\theta_A}\right)} \tag{130}$$

$$A=\frac{-\left(e^{i\theta_A}-e^{-i\theta_A}\right)\left(e^{-\theta_B}-e^{i\theta_A}\right)e^{-2N\theta_B}}{\left(e^{-\theta_B}-e^{-i\theta_A}\right)\left(e^{\theta_B}-e^{i\theta_A}\right)-e^{-2N\theta_B}\left(e^{-\theta_B}-e^{i\theta_A}\right)\left(e^{\theta_B}-e^{-i\theta_A}\right)}\,. \tag{131}$$

Once A and B are known, t and r can be obtained in a straightforward (if slightly tedious) manner:

$$te^{iN\theta_A}=\frac{\left(e^{i\theta_A}-e^{-i\theta_A}\right)\left(e^{\theta_B}-e^{-\theta_B}\right)}{\left(e^{-\theta_B}-e^{-i\theta_A}\right)\left(e^{\theta_B}-e^{i\theta_A}\right)e^{N\theta_B}-\left(e^{-\theta_B}-e^{i\theta_A}\right)\left(e^{\theta_B}-e^{-i\theta_A}\right)e^{-N\theta_B}} \tag{132}$$

$$re^{-i\theta_A}=\frac{\left(e^{\theta_B}+e^{-\theta_B}-e^{i\theta_A}-e^{-i\theta_A}\right)\left(e^{N\theta_B}-e^{-N\theta_B}\right)}{\left(e^{-\theta_B}-e^{-i\theta_A}\right)\left(e^{\theta_B}-e^{i\theta_A}\right)e^{N\theta_B}-\left(e^{-\theta_B}-e^{i\theta_A}\right)\left(e^{\theta_B}-e^{-i\theta_A}\right)e^{-N\theta_B}}\,. \tag{133}$$

Equations (132) and (133) can also be written as,

$$te^{iN\theta_A}=\frac{4i\sin\theta_A\sinh\theta_B}{4\sinh\left(N\theta_B\right)\left[1-\cos\theta_A\cosh\theta_B\right]+4i\cosh\left(N\theta_B\right)\sin\theta_A\sinh\theta_B} \tag{134}$$

and

$$re^{-i\theta_A} = \frac{4\left(\cosh\theta_B - \cos\theta_A\right)\sinh\left(N\theta_B\right)}{4\sinh\left(N\theta_B\right)\left[1-\cos\theta_A\cosh\theta_B\right] + 4i\cosh\left(N\theta_B\right)\sin\theta_A\sinh\theta_B}. \qquad (135)$$

We can make contact with the transmission and reflection amplitudes calculated for the simple barrier model, Equations (43 and 44) by taking advantage of the fact that tight-binding bands have free electron-like dispersion near the top or bottom of the band. Thus we can recover the simple-barrier tunneling amplitude expressions in the following limit,

$$\theta_A = ka \to 0, \quad \sin\theta_A \to \theta_A, \quad \cos\theta_A \to 1 - \frac{1}{2}\theta_A^2 \qquad (136)$$

$$\theta_B = k'a \to 0, \quad \sinh\theta_B \to \theta_B, \quad \cosh\theta_B \to 1 + \frac{1}{2}\theta_B^2 \qquad (137)$$

$$Na = d\,. \qquad (138)$$

Then

$$te^{iN\theta_A} \to \frac{2ikk'}{\left(k^2 - k'^2\right)\sinh\left(k'd\right) + 2ikk'\cosh\left(k'd\right)} \qquad (139)$$

and

$$re^{-i\theta_A} \to \frac{\left(k^2 + k'^2\right)\sinh\left(k'd\right)}{\left(k^2 - k'^2\right)\sinh\left(k'd\right) + 2ikk'\cosh\left(k'd\right)} \,. \tag{140}$$

Equations (139) and (140) can be seen to be the same as Equation (43) and (44) aside from unimportant phase factors.

CHAPTER 3.4: TRANSMISSION PROBABILITY FOR SIMPLE TIGHT-BINDING TUNNELING

The transmission and reflection probabilities can be obtained from equations (134) and (135) respectively,

$$T = t^* t = \frac{\sin^2\theta_A \sinh^2\theta_B}{\sinh^2\left(N\theta_B\right)\left[1-\cos\theta_A\cosh\theta_B\right]^2 + \cosh^2\left(N\theta_B\right)\sin^2\theta_A\sinh^2\theta_B} \qquad (141)$$

$$R = r^* r = \frac{\left(\cosh\theta_B - \cos\theta_A\right)^2 \sinh^2\left(N\theta_B\right)}{\sinh^2\left(N\theta_B\right)\left[1-\cos\theta_A\cosh\theta_B\right]^2 + \cosh^2\left(N\theta_B\right)\sin^2\theta_A\sinh^2\theta_B}. \qquad (142)$$

Electron conservation ($R+T=1$) can be verified by noting that by repeated use of the identity, $\cosh^2\theta = 1+\sinh^2\theta$, the common denominator in Equations (141) and (142) can be written as,

$$\begin{aligned}&\sinh^2\left(N\theta_B\right)\left[1-\cos\theta_A\cosh\theta_B\right]^2 + \cosh^2\left(N\theta_B\right)\sin^2\theta_A\sinh^2\theta_B \\ &= \left(\cosh\theta_B - \cos\theta_A\right)^2\sinh^2\left(N\theta_B\right) + \sin^2\theta_A\sinh^2\theta_B.\end{aligned} \qquad (143)$$

Equations (141) and 142) can also be written in a form that shows the energy dependence more clearly, by using $x = \varepsilon - \varepsilon_A = 2\cos\theta_A$ and $y = \varepsilon - \varepsilon_B = z + z^{-1} = 2\cosh\theta_B$ or $2\cos\theta_B$ if $\left|\varepsilon - \varepsilon_B\right| < 2$,

$$R = \frac{\left(x-y\right)^2\left(z^N - z^{-N}\right)^2}{\left(y-x\right)^2\left(z^N - z^{-N}\right)^2 - \left(4-x^2\right)\left(4-y^2\right)} \qquad (144)$$

$$T = \frac{-\left(4-x^2\right)\left(4-y^2\right)}{\left(y-x\right)^2\left(z^N - z^{-N}\right)^2 - \left(4-x^2\right)\left(4-y^2\right)} . \qquad (145)$$

Written in this form, conservation of electrons, $R+T=1$, is immediately obvious. Similarly to the interface case we can make contact with the simple barrier model in a limit in which $\theta_A = ka \to 0$, $\theta_B = k'a \to 0$, and $Na = d$.

$$T = t^* t = \frac{\sin^2\theta_A \sinh^2\theta_B}{\sinh^2\left(N\theta_B\right)\left[1-\cos\theta_A\cosh\theta_B\right]^2 + \cosh^2\left(N\theta_B\right)\sin^2\theta_A\sinh^2\theta_B}$$

$$\to \qquad \frac{\left(2k'k\right)^2}{\left(2k'k\right)^2 + \left(k^2+k'^2\right)^2\sinh^2 k'd}$$

$$R = r^* r = \frac{\left(\cosh\theta_B - \cos\theta_A\right)^2\sinh^2\left(N\theta_B\right)}{\sinh^2\left(N\theta_B\right)\left[1-\cos\theta_A\cosh\theta_B\right]^2 + \cosh^2\left(N\theta_B\right)\sin^2\theta_A\sinh^2\theta_B}$$

$$\to \qquad \frac{\left(k^2+k'^2\right)^2\sinh^2 k'd}{\left(2k'k\right)^2 + \left(k^2+k'^2\right)^2\sinh^2 k'd}$$

This limit can be taken consistently if the energy is very near the top or bottom of the conduction band for the leads and simultaneously just below the bottom or just above the top of the conduction band for the barrier.

The variation of the transmission probability with energy for the A-B-A system is shown in Figures 6 and 7. The A (leads) onsite energy in units of the hopping matrix element is chosen to be 0, and the B (barrier) onsite energy is chosen to be 2. The band of the leads will extend from -2 to 2, the range

over which the figure is plotted. The band of the barrier extends from 0 to 4. There is wave propagation from $\varepsilon = 0$ to $\varepsilon = 2$, energies where propagation is allowed in both leads and barrier. In the region $\varepsilon = -2$ to $\varepsilon = 0$ there is a small transmission due to quantum mechanical tunneling. Figures 6 and 7 show the transmission probability for *N*=10, and 5 respectively, *i.e.* for 10 and 5 B atoms in the barrier.

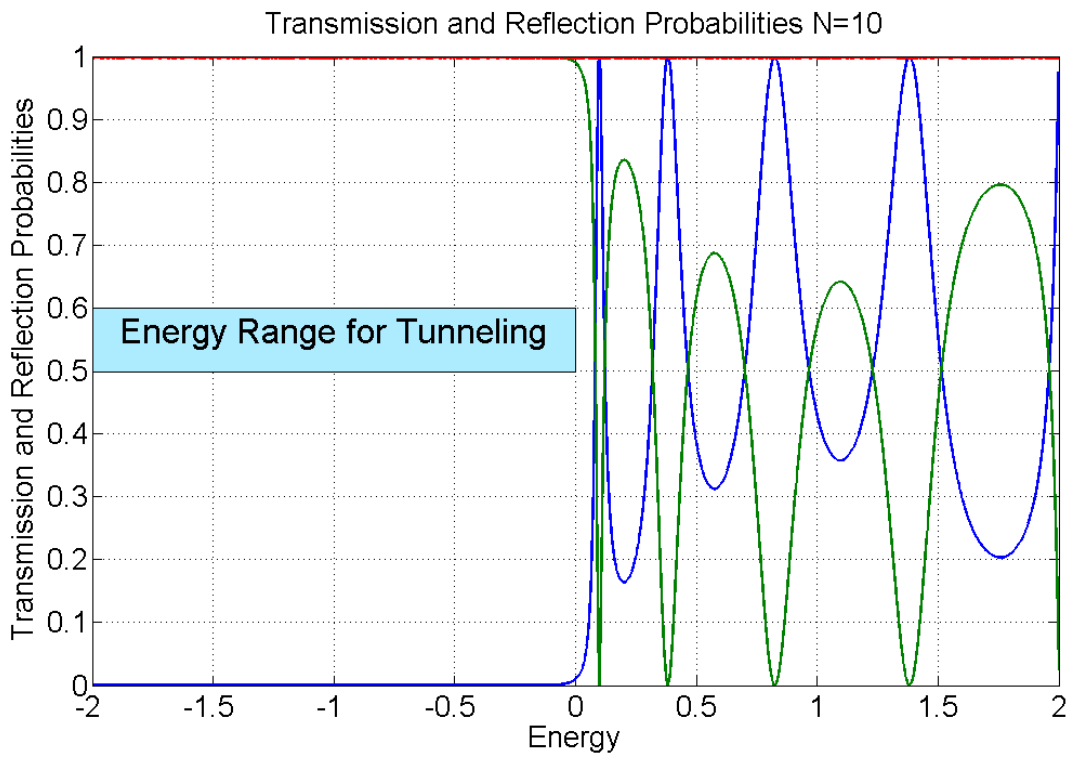

Figure 6: Transmission (blue) and Reflection (green) probabilities for the A-B-A tight-binding model as a function of energy. Parameters are $\varepsilon_A = 0,\ \varepsilon_B = 2,\ N = 10$. Energy is measured in units of hopping matrix element, w . The red curve shows the sum of Transmission and Reflection probabilities.

For some energies in the non-tunneling energy range, the transmission probability reaches 100%. These are energies for which $N\theta_B = m\pi$ where m is an integer. In the non-tunneling or band

conduction regime, the hyperbolic functions in Equation (141) become circular functions. Thus perfect transmission will occur for $\theta_B = m\pi / N$ or for $\varepsilon = \varepsilon_B + 2\cos\left(m\pi / N\right)$.

Figure 7 shows a similar plot of the transmission, but for N=5. It can be seen that the approximately exponential decay of the transmission probability into the barrier is slower for this case than when the barrier is thicker as in Figure 6.

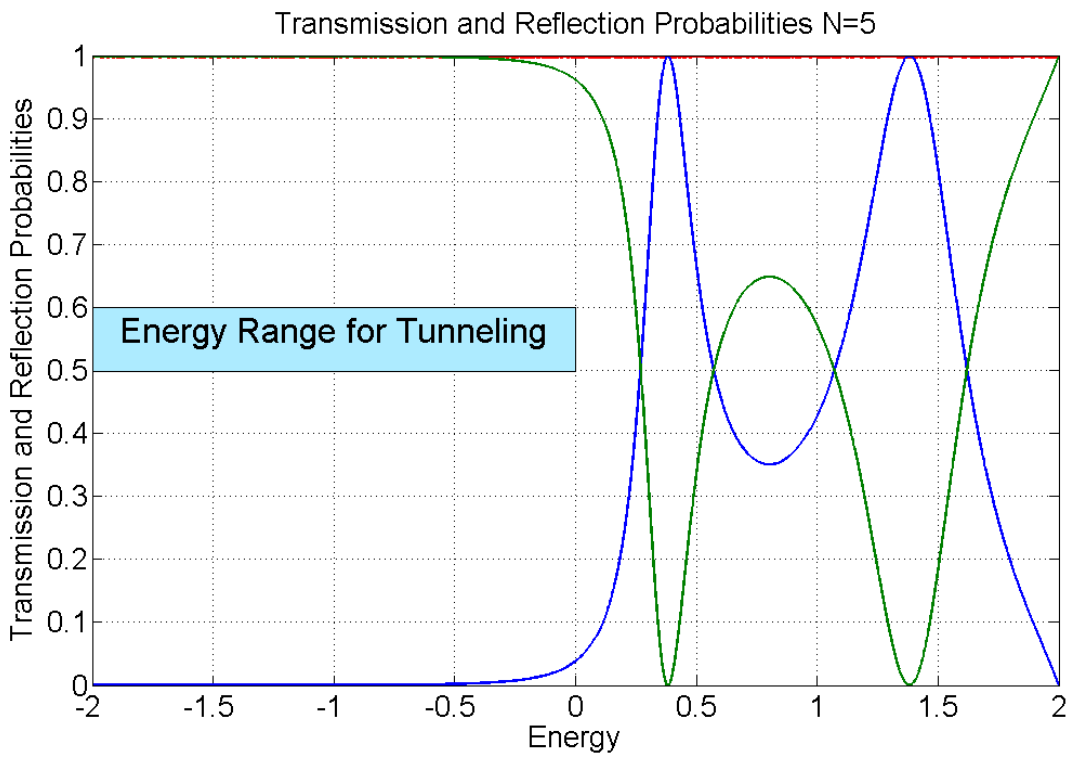

Figure 7: Transmission (blue) and Reflection (green) probabilities for the A-B-A tight-binding model as a function of energy. Parameters are $\varepsilon_A = 0,\ \varepsilon_B = 2,\ N=5$. Energy is measured in units of hopping matrix element, w.

Figure 8 shows the transmission and reflection probabilities using a logarithmic scale so that decay of the tunneling probability can be seen at energies far from the band edge for propagation in the barrier.

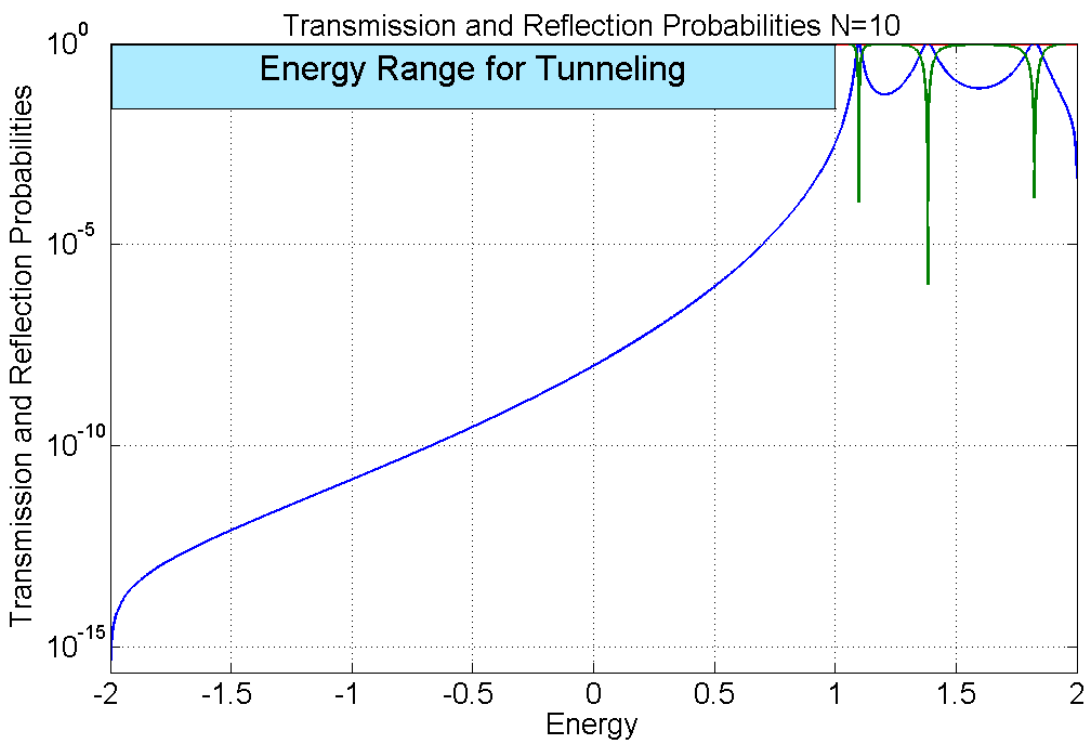

Figure 8: Transmission and Reflection Probabilities plotted with a logarithmic scale. The tight-binding tunneling parameters are $\varepsilon_A = 0,\ \varepsilon_B = 3,\ N = 10.$

Figure 9 shows the wave function at $\varepsilon = 0.99$ using the parameters of Figure 8. The blue and red points (boxes) represent the real and imaginary parts of the wave function coefficients on the atomic sites as described in Equations (106-108). Waves are incident from the left from $-\infty$ and are outgoing on the right toward $+\infty$. Note that the wave function changes sign between

adjacent atoms in the barrier. This is due to $e^{-\theta_B}$ being negative below the bottom of the band for the barrier. If we move the barrier band down so that the energy is above the band maximum for the barrier, the factor $e^{-\theta_B}$ will be greater than zero. This is illustrated in Figure 10 which uses the parameters, $\varepsilon_A = 0,\ \varepsilon_B = -3,\ \varepsilon = -0.99$, so that E is slightly above the B band maximum of 1.

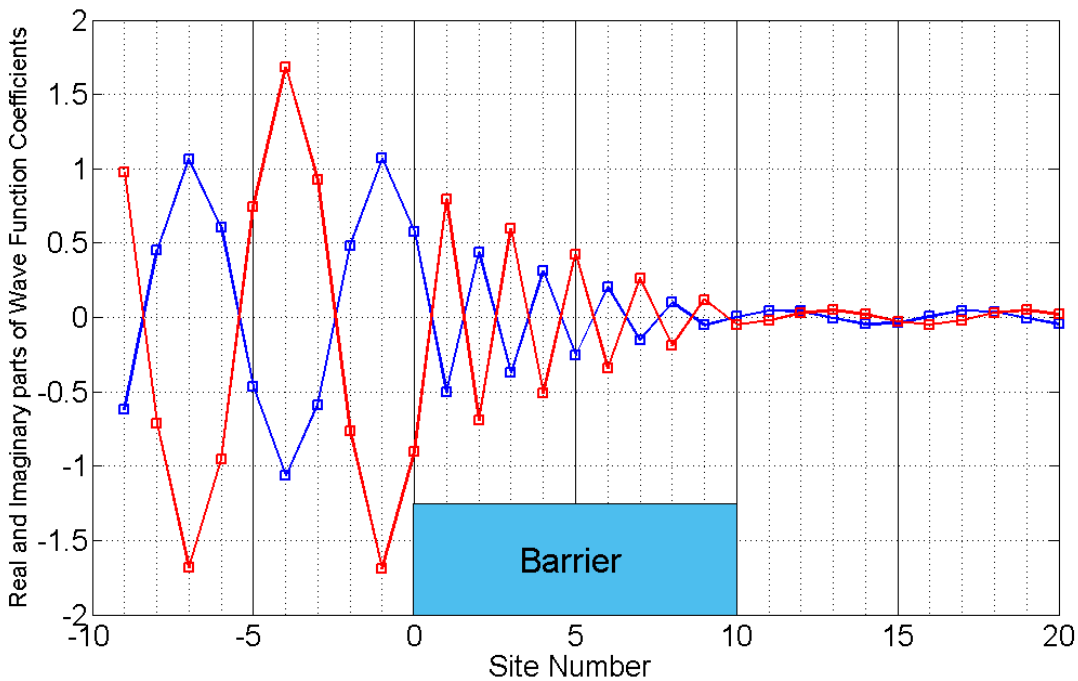

Figure 9: Parameters are $\varepsilon_A = 0,\ \varepsilon_B = 3,\ \varepsilon = -0.99, N = 10.$ The wave function coefficients for the real and imaginary parts of the wave function are shown by the blue and red boxes respectively. The blue and red lines joining the boxes serve as a guide to the eye.

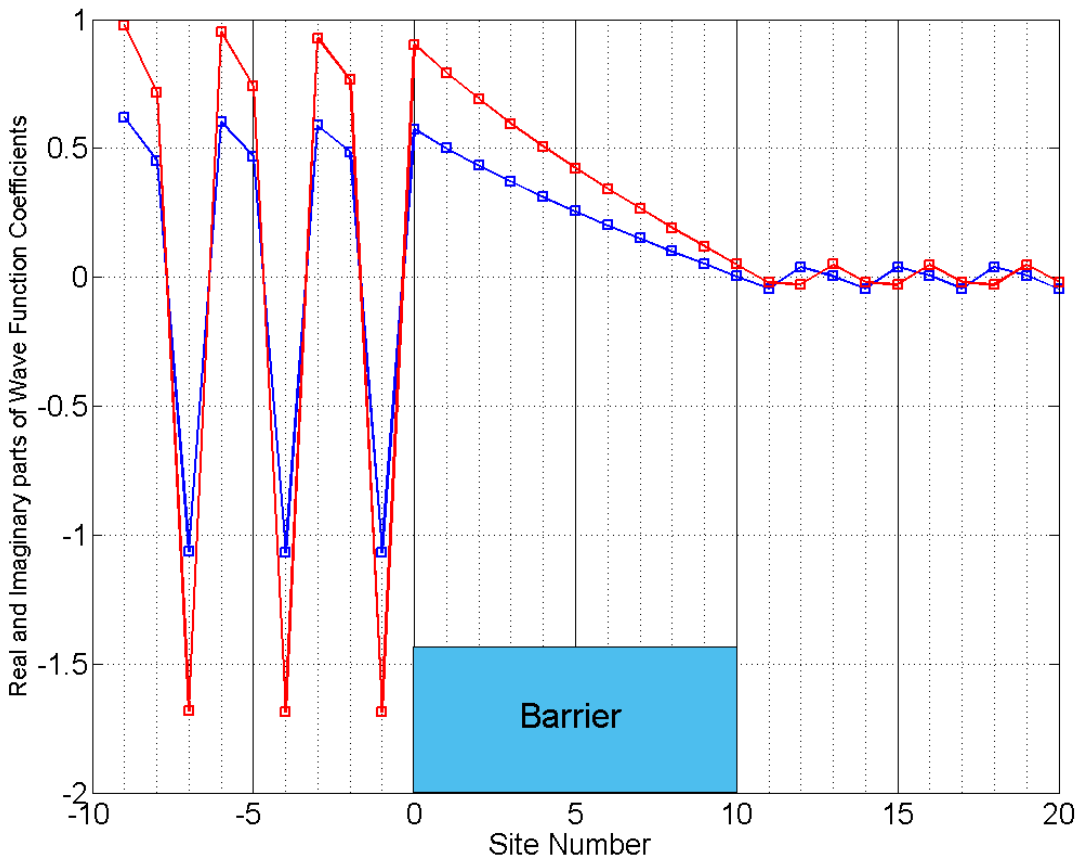

Figure 10: Parameters are $\varepsilon_A = 0,\ \varepsilon_B = -3,\ \varepsilon = -0.99, N = 10.$ The wave function coefficients for the real and imaginary parts of the wave function are shown by the blue and red boxes respectively. The blue and red lines joining the boxes serve as a guide to the eye.

CHAPTER 3.5: CURRENT DENSITY IN TIGHT-BINDING

In order to understand the above results for the transmission and reflection amplitudes, especially the results for the A-B System, we must understand the current in the tight-binding approximation. In analogy to the derivation of the current in Chapter 2 (starting from Equation (57)), we have, for our one dimensional tight-binding model, the time-dependent wave function,

$$\Phi(t) = \sum_n c_n(t)\phi_n \,, \tag{146}$$

which obeys the time dependent Schrödinger equation,

$$i\hbar \frac{\partial}{\partial t}\Phi(t) = H\Phi(t) \,. \tag{147}$$

This can be written in terms of the wave function coefficients by using the assumed orthonormality properties of the local orbitals,

$$i\hbar \frac{\partial}{\partial t} c_n(t) = E_0 c_n(t) + w c_{n+1}(t) + w c_{n-1}(t) \,. \tag{148}$$

The probability that an electron is on site, n, is given by

$$\rho_n(t) = c_n^*(t) c_n(t) \,, \tag{149}$$

and the time derivative of this quantity is given by,

$$i\hbar \frac{\partial}{\partial t}\rho_n(t) = i\hbar\left[c_n \frac{\partial c_n^*}{\partial t} + c_n^* \frac{\partial c_n}{\partial t}\right], \tag{150}$$

but this can be evaluated by use of Equation (143) and its complex conjugate:

$$i\hbar c_n^* \frac{\partial}{\partial t} c_n = E_0 c_n^* c_n + w c_n^* c_{n+1} + w c_n^* c_{n-1} \tag{151}$$

and

$$i\hbar c_n \frac{\partial}{\partial t} c_n^* = -E_0 c_n c_n^* - w c_n c_{n+1}^* - w c_n c_{n-1}^*. \tag{152}$$

Thus the time rate of change of the number of electrons on a site is given by,

$$i\hbar \frac{\partial}{\partial t}\rho_n(t) = \left[\left(w c_n^* c_{n-1} - w c_n c_{n-1}^*\right) - \left(w c_n c_{n+1}^* - w c_n^* c_{n+1}\right)\right], \tag{153}$$

but this must be equal to the difference between the current coming in from the left and the current leaving from the right,

$$\frac{\partial}{\partial t}\rho_n(t) = \frac{i}{\hbar}\left[\left(w c_n c_{n-1}^* - w c_n^* c_{n-1}\right) - \left(w c_n^* c_{n+1} - w c_n c_{n+1}^*\right)\right] = J_{n-\frac{1}{2}} - J_{n+\frac{1}{2}}, \tag{154}$$

where,

$$J_{n-\frac{1}{2}} = \frac{i}{\hbar}\left(w c_n c_{n-1}^* - w c_n^* c_{n-1}\right) \tag{155}$$

and

$$J_{n+\frac{1}{2}} = \frac{i}{\hbar}\left(wc_{n+1}c_n^* - wc_{n+1}^*c_n\right). \tag{156}$$

We are now in a position to discuss the reflection and transmission amplitudes, Equations (106) and (107), in terms of the electron currents. The current on the left is given by substituting Equation (98) into the expression for the current, Equation (98) into one of the expressions for the current, obtaining,

$$J_{Left} = -\frac{2w\sin\theta_A}{\hbar}\left(1 - r^* r\right). \tag{157}$$

Similarly, use of Equation (99) in the expression for the current yields,

$$J_{right} = -\frac{2w\sin\theta_B}{\hbar}t^* t\,. \tag{158}$$

Substituting from the expressions for r and t, (Equations (154) and (155)) allows us to verify that $J_{Left} = J_{right}$. If we define the transmission and reflection probabilities to be,

$$T = \frac{\sin\theta_B}{\sin\theta_A}t^* t \tag{159}$$

and

$$R = r^* r \,, \tag{160}$$

then we have $R + T = 1$ as expected. The reason we need to modify the definition of the transmission probability to include the factor, $\frac{\sin\theta_A}{\sin\theta_B}$, is that the incident and transmitted wave functions have different normalizations, i.e. the current or flux carried by $\exp\left(in\theta_A\right)$ differs from that carried by $\exp\left(in\theta_B\right)$. If we had been careful to include the normalization factors to ensure equality of these fluxes then the additional factor, would not have been needed.

The negative sign in front of the expression for the currents has a simple explanation. $-2wa\sin\theta/\hbar$ is the electron velocity for an electron with dispersion relation $E\left(\theta\right) = E_0 + 2w\cos\theta$. Thus Equation (153) could be written $J_{Right} = vt^* t$ which may be compared to the analogous Equation (75) for the current in the simple barrier problem. When $w > 0$, the energy is a maximum for $\theta = ka = 0$. To compare the simple barrier model with a limiting case of the tight-binding model, we will need to take $w < 0$.

Note that when the energy is outside the range $-2w < E - E_B < 2w$ so that θ_B is imaginary, then the current expressions give zero for the current on the right. This is consistent with $R = 1$ as derived above.

CHAPTER 4: TUNNELING THROUGH A BARRIER WITH A GAP

The systems that we have studied so far, the simple barrier model based on free electron dispersion and the single-orbital tight-binding model differ from realistic tunneling in that neither involve tunneling through a “gap”. In the free-electron based simple barrier model, the barrier is made non-conducting by raising the zero of energy so that it is above the Fermi energy of the leads. In the single-orbital tight binding model, the conduction band of the barrier is positioned so that its minimum is above the Fermi energy or its maximum is below the Fermi energy. In none of these situations is the Fermi energy positioned in a gap between two bands. In this chapter we shall investigate tunneling through a barrier with a gap in its dispersion relation.

CHAPTER 4.1: THE A-[B-C] SYSTEM

A simple way to generate a gap is to have two types of atoms with different on-site orbital energies as shown in Figure 11.

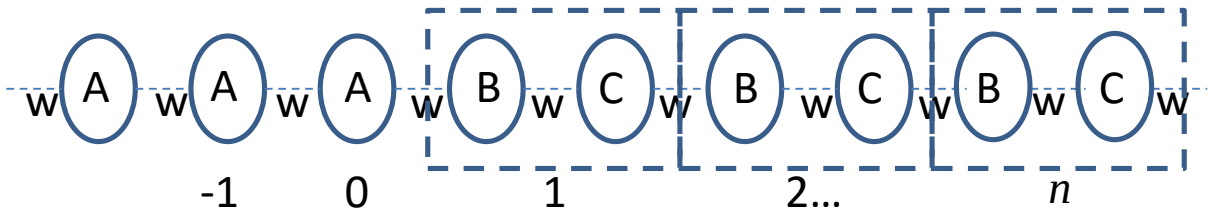

Figure 11: Single s-orbital model – Semi-infinite chains of A atoms and B-C molecules. The A atoms extend from $n=-\infty$ to $n=0$. The B-C molecules extend from $n=1$ to $n=\infty$.

In this system, a semi-infinite chain of A atoms connects on the left to a semi-infinite chain of B-C molecules on the right. The parameters will be chosen such that the A atoms are metallic having a propagating state at the energy, that we will designate as the Fermi energy. The B-C molecules can be designated as an insulator or as a metal, to be determined by us. Importantly for creating a gap, B-C molecules have two different orbitals. For nearest neighbor interactions, there will be a gap between the B and C onsite energies. Let E_A, E_B, and E_C be respectively the on-site energies for the orbitals on sites A, B, and C. For the left part of the A-BC system the wave function ($n<0$) is represented by

$$\psi_{Left} = \sum_{-\infty}^{0} c_n^A \phi_n^A \left(r - R_n\right), \tag{161}$$

$$\psi_{Right} = \sum_{n=1}^{\infty} c_n^B \phi_n^B \left(r - R_n\right) \text{ (B-atoms)}, \tag{162}$$

and

$$\psi_{Right} = \sum_{n=1}^{\infty} c_n^C \phi_n^C \left(r - R_n \right) \quad \text{(C-atoms)}. \tag{163}$$

The Hamiltonian together with the assumed orthonormality of the orbitals will generate an infinite set of equations:

$$\left(E - E_A\right) c_n^A - w\left(c_{n-1}^A + c_{n+1}^A\right) = 0 \ \text{ for } n < 0, \tag{164}$$

$$\left(E - E_A\right) c_n^A - w\left(c_{n-1}^A + c_{n+1}^B\right) = 0 \ \text{ for } n = 0, \tag{165}$$

$$\left(E - E_B\right) c_1^B - w\left(c_0^A + c_1^C\right) = 0 \ \text{ for } n = 1, \tag{166}$$

$$\left(E - E_C\right) c_1^C - w\left(c_1^B + c_2^B\right) = 0 \ \text{ for } n = 1, \tag{167}$$

$$\left(E - E_B\right) c_n^B - w\left(c_{n-1}^A + c_{n+1}^C\right) = 0 \ \text{ for } n > 1, \tag{168}$$

and

$$\left(E - E_C\right) c_n^C - w\left(c_{n-1}^B + c_{n+1}^B\right) = 0 \ \text{ for } n > 1. \tag{169}$$

Note that two equations are needed for each two atom cell for $n > 0$:

The boundary condition on the left in the chain of A atoms is the sum of an incoming, right-going wave of unit amplitude, $e^{in\theta_A}$, and a reflected, left-going wave of amplitude r, $re^{-in\theta_A}$. The boundary condition on the right is a transmitted right-going wave that has amplitude $t_B z^n$ on the B atoms and $t_C z^n$ on the C atoms. Using these boundary conditions and defining, $E = w\varepsilon$, $E_A = w\varepsilon_A$, $E_B = w\varepsilon_B$, $E_C = w\varepsilon_c$, we have from Equation (164), $\varepsilon - \varepsilon_A = 2\cos\theta_A$,and from Equations (168) and (169) using $c_{n+1}^B = zc_n^B$, $c_{n+1}^C = zc_n^C$,

$$\begin{bmatrix} \varepsilon - \varepsilon_B & -\left(1 + z^{-1}\right) \\ -\left(1 + z\right) & \varepsilon - \varepsilon_C \end{bmatrix} \begin{bmatrix} t_B \\ t_C \end{bmatrix} = 0, \tag{170}$$

which implies that,

$$\left(\varepsilon - \varepsilon_B\right)\left(\varepsilon - \varepsilon_C\right) = z + z^{-1} + 2. \tag{171}$$

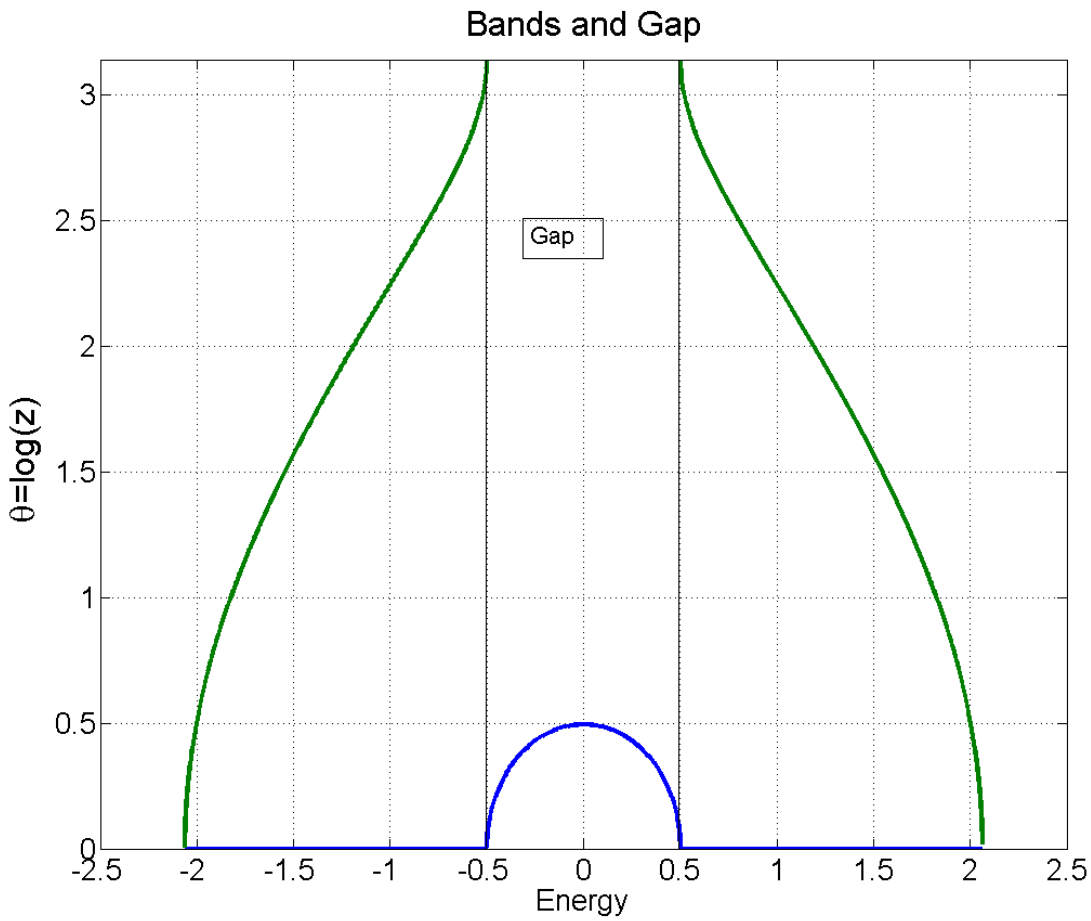

Figure 12: Dispersion relation for B-C chain. A gap extends from $\varepsilon_B = -0.5$ to $\varepsilon_C = 0.5$. Blue and green curves are real and imaginary parts of log(z) respectively where $(\varepsilon - \varepsilon_B)(\varepsilon - \varepsilon_C) = z + \frac{1}{z} + 2$.

On substitution of boundary conditions, Equation (165) becomes,

$$(\varepsilon - \varepsilon_A)(1 + r) - \left(e^{-i\theta_A} + re^{i\theta_A} + t_B z\right) = 0, \tag{172}$$

which, with the help of the results from Equation (164) can be written as,

$$r - t_B z e^{i\theta_A} = -e^{2i\theta_A} \tag{173}$$

Similarly, Equation (167) becomes,

$$\left(\varepsilon - \varepsilon_C\right) t_C z - t_B z \left(1 + z\right) = 0\,, \tag{174}$$

which allows us to write,

$$t_C = \frac{t_B \left(1 + z\right)}{\left(\varepsilon - \varepsilon_C\right)}\,. \tag{175}$$

and Equation (166) becomes

$$\left(\varepsilon - \varepsilon_B\right) t_B z - \left(1 + r + t_C z\right) = 0\,, \tag{176}$$

which with the use of Equations (171) and (173), may be written as,

$$-r + \left[\frac{1 + z^{-1}}{\left(\varepsilon - \varepsilon_C\right)}\right] t_B z = 1\,. \tag{177}$$

Adding Equations (173) and (177) yields a solution for t_B,

$$t_B z = \frac{\left(1 - e^{2i\theta_A}\right)\left(\varepsilon - \varepsilon_C\right)}{1 + z^{-1} - \left(\varepsilon - \varepsilon_C\right) e^{i\theta_A}}\,, \tag{178}$$

from which a solution for t_C follows,

$$t_C z = \frac{\left(1-e^{2i\theta_A}\right)\left(1+z\right)}{1+z^{-1}-\left(\varepsilon-\varepsilon_C\right)e^{i\theta_A}}, \tag{179}$$

as well as a solution for r, (using Equation (176)),

$$r = -\frac{\left(\varepsilon-\varepsilon_C\right)-\left(1+z^{-1}\right)e^{i\theta_A}}{\left(\varepsilon-\varepsilon_C\right)-\left(1+z^{-1}\right)e^{-i\theta_A}}. \tag{180}$$

The reflection probability, $R = r^* r$, is clearly unity if z is real, i.e. if the parameters are such as to forbid conduction in the B-C chain. However, if $z = e^{i\theta_{BC}}$, then R becomes,

$$R = r^* r = \frac{\left(\varepsilon-\varepsilon_C\right)^2+2+2\cos\theta_{BC}-\left(\varepsilon-\varepsilon_C\right)2\cos\theta_A-\left(\varepsilon-\varepsilon_C\right)2\cos\left(\theta_A-\theta_{BC}\right)}{\left(\varepsilon-\varepsilon_C\right)^2+2+2\cos\theta_{BC}-\left(\varepsilon-\varepsilon_C\right)2\cos\theta_A-\left(\varepsilon-\varepsilon_C\right)2\cos\left(\theta_A+\theta_{BC}\right)}. \tag{181}$$

In order to investigate the transmission probability, it is necessary to calculate the current on the right of the interface and compare it to the current carried by the incident wave. An expression for the current is given by Equation (156). This expression involves the wave function coefficients in adjacent atoms of the chain. The easiest place to apply this expression for the B-C chain is between the B and C atoms in one of the cells,

$$J_{n+\frac{1}{2}} = \frac{iw}{\hbar}\left(c_{n+1}c_n^* - c_{n+1}^* c_n\right) = \frac{iw}{\hbar}\left(t_C t_B^* - t_C^* t_B\right). \tag{182}$$

Substituting from Equations (178) and (179) gives,

$$J_{Right} = \frac{iw}{\hbar}\left(\begin{array}{l} \dfrac{\left(1-e^{2i\theta_A}\right)\left(1+z^{-1}\right)}{1+z^{-1}-\left(\varepsilon-\varepsilon_C\right)e^{i\theta_A}}\left(\dfrac{\left(1-e^{2i\theta_A}\right)\left(\varepsilon-\varepsilon_C\right)z^{-1}}{1+z^{-1}-\left(\varepsilon-\varepsilon_C\right)e^{i\theta_A}}\right)^* \\ -\left(\dfrac{\left(1-e^{2i\theta_A}\right)\left(1+z^{-1}\right)}{1+z^{-1}-\left(\varepsilon-\varepsilon_C\right)e^{i\theta_A}}\right)^* \dfrac{\left(1-e^{2i\theta_A}\right)\left(\varepsilon-\varepsilon_C\right)z^{-1}}{1+z^{-1}-\left(\varepsilon-\varepsilon_C\right)e^{i\theta_A}} \end{array}\right). \tag{183}$$

If z is real, Equation (183) gives 0, however if $z = e^{i\theta_{BC}}$, the current is finite and is given by,

$$J_{Right} = \frac{-w}{\hbar}\frac{8\sin^2\theta_A \sin\theta_{BC}\left(\varepsilon-\varepsilon_C\right)}{2+2\cos\theta_{BC}+\left(\varepsilon-\varepsilon_C\right)^2-\left(\varepsilon-\varepsilon_C\right)\left[2\cos\theta_A+2\cos\left(\theta_A+\theta_{BC}\right)\right]}. \tag{184}$$

Both Equations (181) and (184) can be simplified by using, Equation (174) in the form,

$2+2\cos\theta_{BC} = \left(\varepsilon-\varepsilon_B\right)\left(\varepsilon-\varepsilon_C\right)$ giving,

$$R = \frac{\left(\varepsilon-\varepsilon_C\right)+\left(\varepsilon-\varepsilon_B\right)-2\cos\theta_A-2\cos\left(\theta_A-\theta_{BC}\right)}{\left(\varepsilon-\varepsilon_C\right)+\left(\varepsilon-\varepsilon_B\right)-2\cos\theta_A-2\cos\left(\theta_A+\theta_{BC}\right)} \tag{185}$$

and

$$J_{Right} = \frac{-w}{\hbar}\frac{8\sin^2\theta_A \sin\theta_{BC}}{\left(\varepsilon-\varepsilon_B\right)+\left(\varepsilon-\varepsilon_C\right)-2\cos\theta_A-2\cos\left(\theta_A+\theta_{BC}\right)}. \tag{186}$$

The current carried by the incident wave is given by $J_{in} = -2w\sin\theta_A/\hbar$, so that the transmission probability is

$$T = \frac{J_{Right}}{J_{in}} = \frac{4\sin\theta_A \sin\theta_{BC}}{\left(\varepsilon - \varepsilon_B\right) + \left(\varepsilon - \varepsilon_C\right) - 2\cos\theta_A - 2\cos\left(\theta_A + \theta_{BC}\right)} \,. \tag{187}$$

It is now possible to confirm that the sum of R in Equation (185) and T in Equation (187) is unity.

CHAPTER 4.2: THE A-[B-C] SYSTEM WITH *s-p* BARRIER

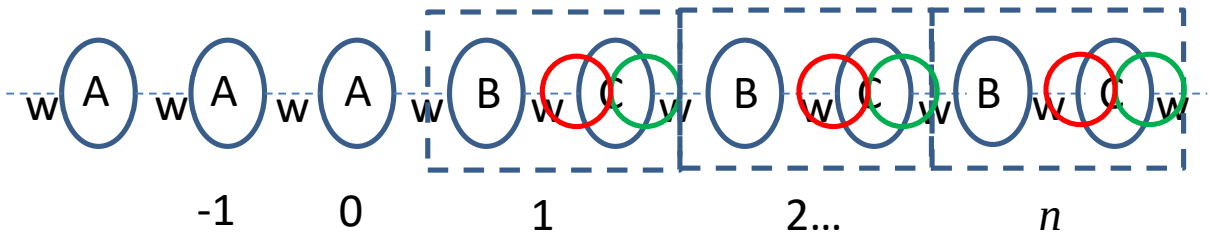

Figure 13: Single s-p-orbital model – semi-infinite chains of A and B-C molecules. The A atoms extend from $n=-\infty$ to $n=0$. The B-C molecules extend from $n=1$ to $n=\infty$. The orbital on the C atom has p_x symmetry.

In the A-BC (*s-p*) system, the B-C chain is a chain of two-molecule system B and C with atom B having an *s*-orbital and atom C has a *p*-orbital. The system is solved as follows:

$$(\varepsilon-\varepsilon_A)\mathrm{c}_0^A-(c_{-1}^A+c_1^B)=0 \qquad (n=0), \tag{188}$$

$$(\varepsilon-\varepsilon_B)\mathrm{c}_1^B-(c_0^A-c_1^C)=0 \qquad (n=1,\ \text{B atom}), \tag{189}$$

and

$$(\varepsilon-\varepsilon_C)c_1^C-(-c_1^B+c_2^B)=0 \qquad (n=1,\ \text{C atom}). \tag{190}$$

In the A chain, for $n<0$, we have,

$$\left(\varepsilon-\varepsilon_A\right)c_n^A-\left(c_{n-1}^A+c_{n+1}^A\right)=0, \tag{191}$$

And in the B-C chain, for $n>1$, we have

$$\left(\varepsilon-\varepsilon_B\right)c_n^B-\left(c_{n-1}^C-c_n^C\right)=0\,, \tag{192}$$

and

$$\left(\varepsilon-\varepsilon_C\right)c_n^C-\left(c_{n-1}^B-c_n^B\right)=0\,. \tag{193}$$

Equations (192) and (193) lead to the dispersion relation $\left(\varepsilon-\varepsilon_B\right)\left(\varepsilon-\varepsilon_C\right)=z+\frac{1}{z}-2$. The boundary conditions representing an incoming wave from the left and an outgoing wave on the right are

$$c_n^A=e^{in\theta_A}+re^{-in\theta_A}\qquad\left(n\le 0\right), \tag{194}$$

$$c_n^B=t_B z_R^{n-1}, \tag{195}$$

and

$$c_n^C=t_C z_R^{n-1}, \tag{196}$$

respectively. Substitution of the boundary conditions, Equations (194), (195), and (196), into the interface equations, Equations (188), (189), and (190), yields

$$(\varepsilon-\varepsilon_A)(1+r)-(e^{-i\theta_A}+re^{i\theta_A}+t_B)=0\,, \tag{197}$$

$$(\varepsilon-\varepsilon_B)t_B-(1+r-t_C)=0\,, \tag{198}$$

and

$$(\varepsilon-\varepsilon_C)\,\mathrm{t}_C-(-t_B+t_B z_R)=0\,. \tag{199}$$

Re-arranging as a set of linear equations for variables r, t_B and t_C,

$$\left(\varepsilon-\varepsilon_A-e^{i\theta_A}\right)r-t_B=-\left(\varepsilon-\varepsilon_A-e^{-i\theta_A}\right), \tag{200}$$

$$-r+\left(\varepsilon-\varepsilon_B\right)t_B+t_C=1, \tag{201}$$

and

$$\left(1-z_R\right)t_B+\left(\varepsilon-\varepsilon_c\right)t_C=0\,. \tag{202}$$

We can use Equation (202), to eliminate t_C,

$$t_C=-\frac{(1-z_R)}{(\varepsilon-\varepsilon_C)}t_B\,, \tag{203}$$

Next, using Equation (191) we obtain, $\varepsilon-\varepsilon_A=e^{i\theta_A}+e^{-i\theta_A}$ which we substitute into Equation (200), so that after substituting Equation (203) into (202), Equations (200) and (201) become

$$\begin{aligned} &r-t_B e^{i\theta_A}=-e^{2i\theta_A} \\ &-r+(\varepsilon-\varepsilon_B)t_B-\frac{(1-z_R)}{(\varepsilon-\varepsilon_C)}t_B=1 \end{aligned}. \tag{204}$$

The sum of the two equations (204) gives,

$$\left[(\varepsilon-\varepsilon_B-e^{i\theta_A})(\varepsilon-\varepsilon_C)-(1-z_R)\right]t_B=(1-e^{2i\theta_A})(\varepsilon-\varepsilon_C)\,. \tag{205}$$

Then one can solve Equation (205) for t_B and use Equation (203) to obtain t_C,

$$\begin{aligned} t_B &= \frac{(1-e^{2i\theta_A})(\varepsilon-\varepsilon_C)}{(\varepsilon-\varepsilon_B-e^{i\theta_A})(\varepsilon-\varepsilon_C)-(1-z_R)}, \\ t_C &= \frac{-(1-e^{2i\theta_A})(1-z_R)}{(\varepsilon-\varepsilon_B-e^{i\theta_A})(\varepsilon-\varepsilon_C)-(1-z_R)}. \end{aligned} \tag{206}$$

With an equation for t_B, either of Equations (204) can be used to obtain r,

$$re^{-i\theta_A}=-e^{i\theta_A}+t_B=\frac{(1-e^{2i\theta_A})(\varepsilon-\varepsilon_C)}{(\varepsilon-\varepsilon_B-e^{i\theta_A})(\varepsilon-\varepsilon_C)-(1-z_R)}-e^{i\theta_A}\,. \tag{207}$$

We rearrange Equation (207) to get

$$\begin{aligned} re^{-2i\theta_A} &= \frac{(e^{-i\theta_A}-e^{i\theta_A})(\varepsilon-\varepsilon_C)-(\varepsilon-\varepsilon_B-e^{i\theta_A})(\varepsilon-\varepsilon_C)+(1-z_R)}{(\varepsilon-\varepsilon_B-e^{i\theta_A})(\varepsilon-\varepsilon_C)-(1-z_R)} \\ &= -\frac{(\varepsilon-\varepsilon_B-e^{-i\theta_A})(\varepsilon-\varepsilon_C)-(1-z_R)}{(\varepsilon-\varepsilon_B-e^{i\theta_A})(\varepsilon-\varepsilon_C)-(1-z_R)}, \end{aligned} \tag{208}$$

and r is given by

$$r=-\frac{(\varepsilon-\varepsilon_B-e^{-i\theta_A})(\varepsilon-\varepsilon_C)-(1-z_R)}{(\varepsilon-\varepsilon_B-e^{i\theta_A})(\varepsilon-\varepsilon_C)-(1-z_R)}e^{2i\theta_A}\,. \tag{209}$$

If z_R is real, then

$$r*r=\left[-\frac{(\varepsilon-\varepsilon_B-e^{i\theta_A})(\varepsilon-\varepsilon_C)-(1-z_R)}{(\varepsilon-\varepsilon_B-e^{-i\theta_A})(\varepsilon-\varepsilon_C)-(1-z_R)}e^{-2i\theta_A}\right]$$
$$\times\left[-\frac{(\varepsilon-\varepsilon_B-e^{-i\theta_A})(\varepsilon-\varepsilon_C)-(1-z_R)}{(\varepsilon-\varepsilon_B-e^{i\theta_A})(\varepsilon-\varepsilon_C)-(1-z_R)}e^{2i\theta_A}\right]=1. \qquad (210)$$

Thus when the Bloch factor in the B-C region is real indicating that states cannot propagate, the reflection probability is unity. Similarly, it can be seen that the current in the B-C chain obtained by evaluating Equation (182) vanishes. On the other hand, if $z_R \to e^{i\theta_{BC}}$, then

$$R=r^*r=\frac{\varepsilon-\varepsilon_B+\varepsilon-\varepsilon_C-2\cos\theta_A+2\cos\left(\theta_A-\theta_{BC}\right)}{\varepsilon-\varepsilon_B+\varepsilon-\varepsilon_C-2\cos\theta_A+2\cos\left(\theta_A+\theta_{BC}\right)} \qquad (211)$$

and

$$T=\frac{-4\sin\theta_A\sin\theta_{BC}}{\varepsilon-\varepsilon_B+\varepsilon-\varepsilon_C-2\cos\theta_A+2\cos\left(\theta_A+\theta_{BC}\right)}. \qquad (212)$$

The negative sign in the numerator of the transmission indicates that $\sin\theta_A$ and $\sin\theta_{BC}$ have opposite signs.

CHAPTER 4.3: THE A-[B-C]-A – A TUNNELING SYSTEM

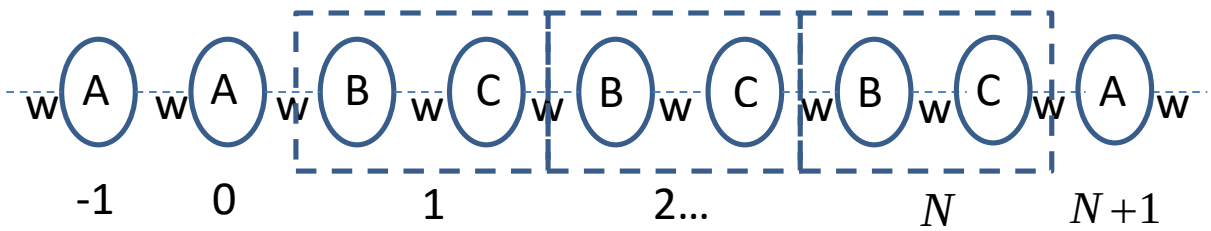

Figure 14: Semi-infinite chain of A atoms on the right and a semi-infinite chain of B atoms on the left. The B-C barrier has orbitals of similar symmetry on the B atom and on the C atom. All inter-atom hopping is assumed to be nearest-neighbor and the same throughout the chain.

The energy dispersion in the leads, is as before, $\varepsilon - \varepsilon_A = 2\cos\theta_A$ and the dispersion relation in the B-C barrier is given by,

$$\left(\varepsilon - \varepsilon_B\right)\left(\varepsilon - \varepsilon_C\right) = 2 + z + \frac{1}{z}. \tag{213}$$

The equations for the two interfaces are, on the left,

$$(\varepsilon - \varepsilon_A)c_0^A - (c_{-1}^A + c_1^B) = 0 \quad \left(\text{for } n = 0\right), \tag{214}$$

$$(\varepsilon - \varepsilon_B)c_1^B - (c_0^A + c_1^C) = 0 \;\; \left(\text{for } n = 1,\ \text{atom B}\right), \tag{215}$$

$$(\varepsilon - \varepsilon_C)c_1^C - (c_1^B + c_2^B) = 0 \;\; \left(\text{for } n = 1,\ \text{atom C}\right), \tag{216}$$

and on the right,

$$(\varepsilon-\varepsilon_B)c_N^B-(c_N^C+c_{N-1}^C)=0 \quad \left(\text{for } n=N \text{ atom B}\right), \tag{217}$$

$$(\varepsilon-\varepsilon_C)c_N^C-(c_N^B+c_{N+1}^A)=0 \quad \left(\text{for } n=N \text{ atom C}\right), \tag{218}$$

and

$$(\varepsilon-\varepsilon_A)c_{N+1}^A-(c_N^C+c_{N+2}^A)=0 \quad \left(\text{for } n=N+1\right). \tag{219}$$

The boundary conditions appropriate to an incident and reflected wave on the left and a transmitted wave on the right with exponentially increasing and decreasing solutions in the barrier are,

$$c_n^A=e^{in\theta_A}+re^{-in\theta_A} \quad \left(n\le 0\right), \tag{220}$$

$$c_n^B=B_+z^n+B_-z^{-n} \quad \left(0<n\le N\right), \tag{221}$$

$$c_n^C=C_+z^n+C_-z^{-n} \quad \left(0<n\le N\right), \tag{222}$$

$$c_n^A=te^{in\theta_A} \quad \left(n\ge N+1\right). \tag{223}$$

Substitution of these boundary conditions into interface equations, gives a set of six equations for the six unknowns r, t, B_+, B_-, C_+, and C_-:

$$(\varepsilon-\varepsilon_A)\left(1+r\right)-(e^{-i\theta_A}+re^{i\theta_A}+B_+z+B_-z^{-1})=0\,, \tag{224}$$

$$(\varepsilon-\varepsilon_B)\left(B_+z+B_-z^{-1}\right)-(1+r+C_+z+C_-z^{-1})=0\,, \tag{225}$$

$$(\varepsilon-\varepsilon_C)\left(C_+z+C_-z^{-1}\right)-(B_+z+B_-z^{-1}+B_+z^2+B_-z^{-2})=0\,, \tag{226}$$

$$(\varepsilon-\varepsilon_B)\left(B_+z^N+B_-z^{-N}\right)-(C_+z^N+C_-z^{-N}+C_+z^{N-1}+C_-z^{-N+1})=0\,, \tag{227}$$

$$(\varepsilon-\varepsilon_C)\left(C_+z^N+C_-z^{-N}\right)-(B_+z^N+B_-z^{-N}+te^{i(N+1)\theta_A})=0\,, \tag{228}$$

and

$$(\varepsilon-\varepsilon_A)te^{i(N+1)\theta_A}-(C_+z^N+C_-z^{-N}+te^{i(N+2)\theta_A})=0\,. \tag{229}$$

These equations will look slightly simpler if, instead of B_+, B_-, C_+, and C_- we use,

$$B_1=\left(B_+z+B_-z^{-1}\right), \tag{230}$$

$$B_N=\left(B_+z^N+B_-z^{-N}\right), \tag{231}$$

$$C_1 = \left(C_+ z + C_- z^{-1}\right), \tag{232}$$

and

$$C_N = \left(C_+ z^N + C_- z^{-N}\right). \tag{233}$$

Once B_1, B_N, C_1, and C_N have been determined, we can find B_+, B_-, C_+, and C_- using,

$$B_+ = \frac{zB_1 - z^N B_N}{z^2 - z^{2N}}, \tag{234}$$

$$B_- = \frac{z^{-1}B_1 - z^{-N} B_N}{z^{-2} - z^{-2N}}, \tag{235}$$

$$C_+ = \frac{zC_1 - z^N C_N}{z^2 - z^{2N}}, \tag{236}$$

and

$$C_- = \frac{z^{-1}C_1 - z^{-N} C_N}{z^{-2} - z^{-2N}}. \tag{237}$$

Our system of six equations becomes

$$(\varepsilon - \varepsilon_A)\left(1 + r\right) - (e^{-i\theta_A} + re^{i\theta_A} + B_1) = 0, \tag{238}$$

$$(\varepsilon - \varepsilon_B)B_1 - (1 + r + C_1) = 0, \tag{239}$$

$$(\varepsilon-\varepsilon_C)C_1-(B_1+B_+z^2+B_-z^{-2})=0\,, \tag{240}$$

$$(\varepsilon-\varepsilon_B)B_N-(C_N+C_+z^{N-1}+C_-z^{-N+1})=0\,, \tag{241}$$

$$(\varepsilon-\varepsilon_C)C_N-(B_N+te^{i(N+1)\theta_A})=0\,, \tag{242}$$

$$(\varepsilon-\varepsilon_A)te^{i(N+1)\theta_A}-(C_N+te^{i(N+2)\theta_A})=0\,. \tag{243}$$

Equations (238) and (243) can be simplified using the dispersion relation for the A chain:

$$r=B_1e^{i\theta_A}-e^{2i\theta_A} \tag{244}$$

and

$$t=C_Ne^{-iN\theta_A}\,. \tag{245}$$

These equations can be used to eliminate r and t leaving equations (239-242) that only involve B_1, C_1, B_N, and C_N:

$$\left(\varepsilon-\varepsilon_B-e^{i\theta_A}\right)B_1-C_1=1-e^{2i\theta_A}\,, \tag{246}$$

$$-\left(1+\frac{z^{N-2}-z^{-N+2}}{z^{N-1}-z^{-N+1}}\right)B_1+\left(\frac{z^{-1}-z}{z^{N-1}-z^{-N+1}}\right)B_N+(\varepsilon-\varepsilon_C)C_1=0\,, \tag{247}$$

$$(\varepsilon-\varepsilon_B)B_N-\left(\frac{z-z^{-1}}{z^{N-1}-z^{-N+1}}\right)C_1-\left(1+\frac{z^{N-2}-z^{-N+2}}{z^{N-1}-z^{-N+1}}\right)C_N=0\,, \tag{248}$$

and

$$-B_N+\left(\varepsilon-\varepsilon_C-e^{i\theta_A}\right)C_N=0\,. \tag{249}$$

These equations can be written in more compact form if we let $b=\varepsilon-\varepsilon_B-e^{i\theta_A}$, $c=\varepsilon-\varepsilon_C-e^{i\theta_A}$, and define $x_n=z^n-z^{-n}$:

$$C_1=bB_1+2i\sin\theta_A e^{i\theta_A}\,, \tag{250}$$

$$-\left(x_{N-1}+x_{N-2}\right)B_1-x_1B_N+(\varepsilon-\varepsilon_C)x_{N-1}C_1=0\,, \tag{251}$$

$$(\varepsilon-\varepsilon_B)x_{N-1}B_N-x_1C_1-\left(x_{N-1}+x_{N-2}\right)C_N=0\,, \tag{252}$$

and

$$B_N=cC_N\,. \tag{253}$$

Equations (250) and (253) can be used to eliminate C_1 and B_N, leaving two equations for the remaining two unknowns, B_1 and C_N:

$$-\left(x_{N-1}+x_{N-2}-x_{N-1}(\varepsilon-\varepsilon_C)b\right)B_1-x_1cC_N=-2i\sin\theta_A e^{i\theta_A}(\varepsilon-\varepsilon_C)x_{N-1} \tag{254}$$

and

$$-x_1bB_1-\left(x_{N-1}+x_{N-2}-x_{N-1}(\varepsilon-\varepsilon_B)c\right)C_N=x_1 2i\sin\theta_A e^{i\theta_A}. \tag{255}$$

The coefficients of B_1 in Equation (254) and of C_N in Equation (255) may be simplified, using, for example,

$$\begin{aligned} &x_{N-1}+x_{N-2}-x_{N-1}(\varepsilon-\varepsilon_C)b \\ &\quad=x_{N-1}+x_{N-2}-x_{N-1}\left(2+z+z^{-1}-(\varepsilon-\varepsilon_C)e^{i\theta_A}\right) \\ &\quad=-\left(x_N-c^*e^{i\theta_A}x_{N-1}\right). \end{aligned} \tag{256}$$

Equations (254) and (255) for B_1 and C_N become,

$$\left(x_N-c^*e^{i\theta_A}x_{N-1}\right)B_1-x_1cC_N=-2i\sin\theta_A e^{i\theta_A}(\varepsilon-\varepsilon_C)x_{N-1} \tag{257}$$

$$-x_1bB_1+\left(x_N-b^*e^{i\theta_A}x_{N-1}\right)C_N=x_1 2i\sin\theta_A e^{i\theta_A}. \tag{258}$$

Equation (258) can be solved for B_1:

$$B_1=-2i\sin\theta_A e^{i\theta_A}b^{-1}+x_1^{-1}b^{-1}\left(x_N-b^*e^{i\theta_A}x_{N-1}\right)C_N. \tag{259}$$

Then Equation (257) yields a solution for C_N and t

$$C_N=-2ix_1\sin\theta_A e^{i\theta_A}\frac{\left[b(\varepsilon-\varepsilon_C)x_{N-1}-\left(x_N-c^*e^{i\theta_A}x_{N-1}\right)\right]}{\left[\left(x_N-b^*e^{i\theta_A}x_{N-1}\right)\left(x_N-c^*e^{i\theta_A}x_{N-1}\right)-x_1^2cb\right]}=te^{iN\theta_A}. \tag{260}$$

The numerator can be simplified since,

$$\begin{aligned} & b(\varepsilon-\varepsilon_C)x_{N-1}+c^{*}e^{i\theta_A}x_{N-1}-x_N \\ & \quad =(\varepsilon-\varepsilon_B)(\varepsilon-\varepsilon_C)x_{N-1}-x_{N-1}-x_N \\ & \quad =\left(2+z+z^{-1}\right)x_{N-1}-x_{N-1}-x_N=x_{N-1}+x_{N-2}. \end{aligned} \tag{261}$$

Thus, the transmission amplitude can be written as,

$$te^{iN\theta_A}=-2ix_1\sin\theta_A e^{i\theta_A}\frac{x_{N-1}+x_{N-2}}{\left(x_N-b^{*}e^{i\theta_A}x_{N-1}\right)\left(x_N-c^{*}e^{i\theta_A}x_{N-1}\right)-x_1^2cb}. \tag{262}$$

where $b=\varepsilon-\varepsilon_B-e^{i\theta_A}$, $c=\varepsilon-\varepsilon_C-e^{i\theta_A}$, and $x_n=z^n-z^{-n}$.

The transmission probability as a function of energy is shown in Figures 15 – 17.

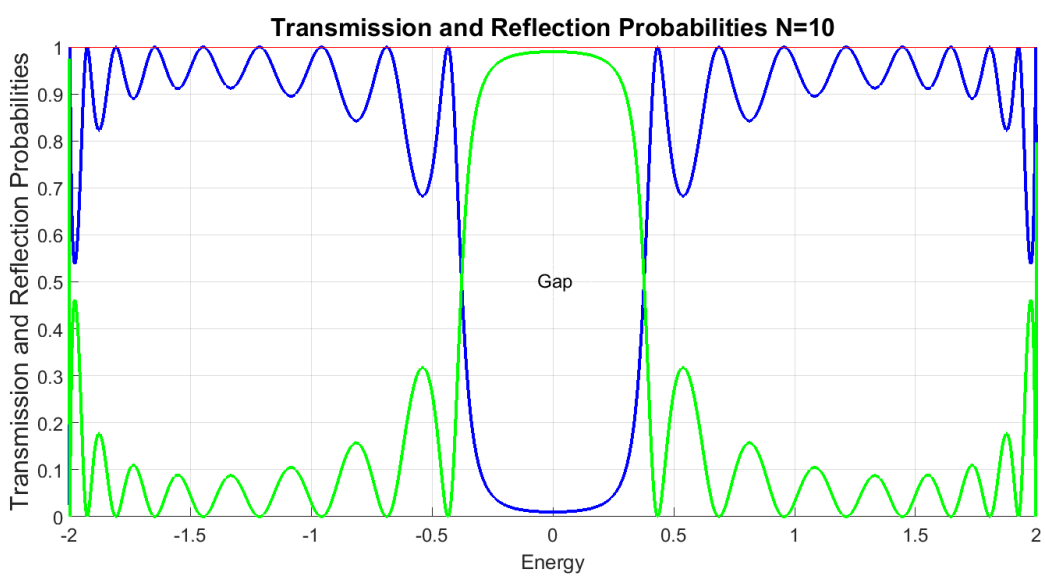

Figure 15: Transmission (blue) and Reflection (green) probabilities for the A-BC-A tight-binding model as a function of energy. Parameters are $\varepsilon_A=0,\ \varepsilon_B=-\varepsilon_C=0.3,\ N=10$. Energy is measured in units of hopping matrix element, w.

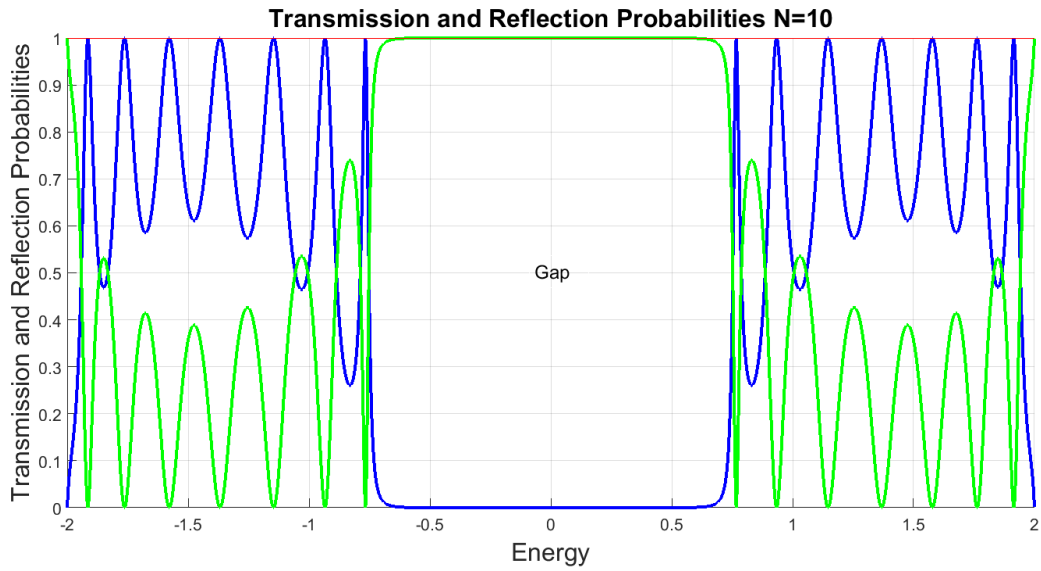

Figure 16: Transmission (blue) and Reflection (green) probabilities for the A-BC-A tight-binding model as a function of energy. Parameters are $\varepsilon_A = 0,\ \varepsilon_B = -\varepsilon_C = 0.7,\ N=10$. Energy is measured in units of hopping matrix element, w .

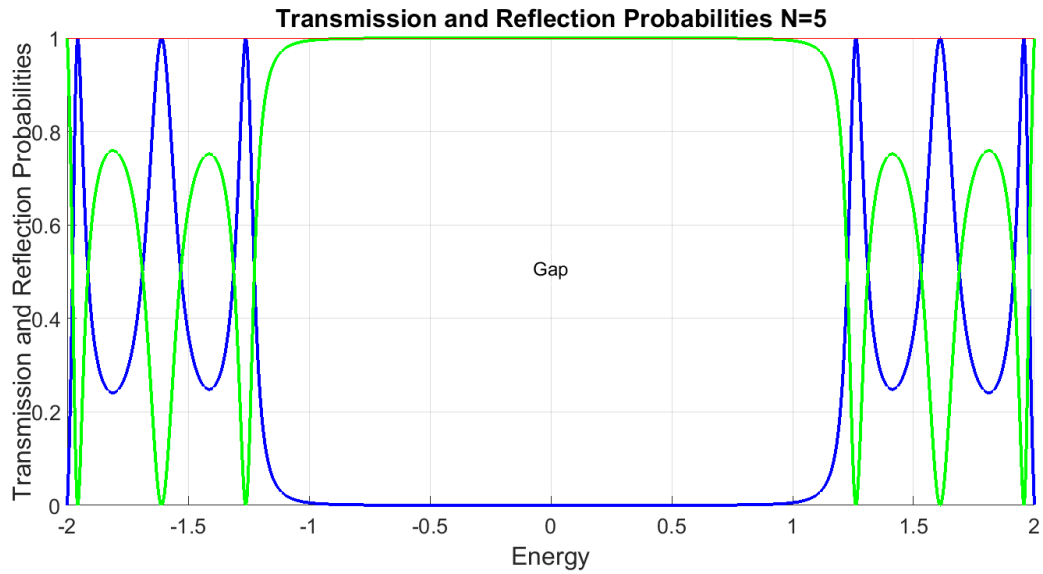

Figure 17: Transmission (blue) and Reflection (green) probabilities for the A-BC-A tight-binding model as a function of energy. Parameters are $\varepsilon_A = 0,\ \varepsilon_B = -\varepsilon_C = 1.1,\ N=5$. Energy is measured in units of hopping matrix element, w .

CHAPTER 5: CONCLUSIONS

We have explored the tunneling properties in quantum mechanical solid state physics. Chapter 2 discusses how we used the Landauer formulation of transport to relate the transmission probability in terms of the conductance and the resistance. Also, the three-dimensional simple barrier model for tunneling was derived using the separation of variables. In order to derive a general expression for the current, we used the separation of variables from the time-dependent formulation of quantum mechanics. Our expression for the current was obtained from the continuity equation.

The simple barrier model for tunneling was solved by calculating the transmission and reflection probabilities. There is a relationship between the transmission probability and the conductance to calculate the conductance of the three dimensional barrier system at low bias. We used our expression for the current density in terms of the wave functions to demonstrate that the current is equal in all three regions of the tunneling system: left lead, barrier, and right lead.

The electron dispersion in solids is not precisely represented due to limitations of the free electron model. This is why we introduce the tight-binding model in Chapter 3. Section 3.2 covers how to calculate transmission and reflection probabilities for an interface using the simplest one-dimensional tight-binding model for an interface between semi-infinite chains of A atoms and B atoms. This model is extended in Section 3.3 to a tunneling system consisting of two semi-infinite chains of A atoms separated by a finite chain of B atoms. We showed that in the limit of very long electron wavelengths and very slow decay of the evanescent states, the tight-binding approximation for tunneling reduces to the simple barrier model in Section 3.4. In Section 3.5, we calculated the transmission and reflection probabilities of the A-B-A model. Section 3.6 covers the energy variation and also the wave functions are plotted to show that

when $E < E_B$, the wave function has the opposite sign on adjacent atoms. In Section 3.7, the current density in the tight-binding approximation was calculated. Then the current density was used to complete the calculation of the transmission probability at an interface.

To produce a dispersion relation with a gap, we cannot use the simple tight-binding model with a single orbital on each site. This is why we continued our calculations to construct a barrier consisting of B-C molecules in Chapter 4. A chain of this type produces a gap extending between the onsite energy for the A atom and the onsite energy for the B atom. Tunneling through gap is calculated and plotted. We have observed that if the orbitals on the B and C atoms have the same parity, the wave function will change sign between molecules, however if the parity of the orbitals are different, there will not be a sign change.

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