THE EFFECTS OF PROPAGATIONAL FACTORS ON QUANTUM WIRES IN CLOSE PARALLEL PROXIMITY

(M.Sc. THESIS)

SUBMITTED BY

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CONTENTS

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I. INTRODUCTION

Recent advances in semiconductor technology have made it possible to produce devices of such small size that electronic conduction through these devices is dominated by the quantum properties of the electron. The fact that an electron travelling through such a device is unaffected by scattering and is able to retain coherence, has received some attention in recent literature [1-3]. The ability to guide an electron wave in quantum wires has in particular opened up opportunities for device applications which are based on the wave nature of the electron.

In this paper we wish to investigate the propagation of an electron wave along the length of two coupled quantum wires. We assume that the wires are sufficiently long and straight, and that they run parallel to each other. These assumptions allow the neglect of the end effects of the wires on the electronic motion and offer considerable simplicity in the calculations. The quantum nature of the wires arises due to smallness of the cross sectional area of the wires which is usually of the order of 100 Angstroms in length in any direction. The wires are defined in terms of two quantum wells such that the electron motion is restricted in the direction transverse to the length of the wire and is unrestricted along its length. We assume that the wires are sufficiently close to each other that an electron wave introduced in one of the wires is able to tunnel itself into the other. The wave could in fact oscillate back and forth between the wires. The frequency of oscillations will depend on the width and depth of the quantum wells and the distance separating the wires. In addition to these parameters, the frequency is also affected by the effective mass of the electron if it is different within and outside the wires [4-5], a situation which can frequently arise. In this situation we will show that the motion of the electrons in the parallel and perpendicular directions become coupled and that the frequency of oscillations of the electron wave depends on the motion of the wave parallel to the wire. It is the main aim of this paper to investigate the effect of the changes in the electron effective mass on the frequency. In addition we wish to obtain the dependence of the frequency on the distance between the wires, and the potential depths and width of the quantum wells.

We assume that the effective mass of the electron within the wires is m_a and outside the wells it is m_s. The potential energy within the two wells is asaumed to be $-V_0$ and zero outside the wells. A schematic diagram representing the system is shown in Fig. 1. The stationary states of the system consist of a plane wave state along the length of the wires and bound and unbound states in a direction normal to the length. We will restrict ourselves in this paper to two bound states only. The wave function in the direction normal to the wire is affected by the wave vector of the plane wave state along the direction of the wire when the mass of the electron is different within and outside the well. The effect vanishes if the mass is the same. In Section II we discuss the effect produced by the difference in the effective mass on the wave function of the electron for a single quantum well. The results would show how the wave function and the energy of the bound state is affected by the electronic motion parallel to the length of the wire. The frequency of oscillations and the stationary state wave functions for an electron bound to two quantum wires is derived using the approach based on the time dependence of the probability amplitudes of occupancy for the electron in one wire or the other. The approach is explained in Section III. The frequency of oscillation of the electron wave is obtained in Section IV and the numerical results are obtained and discussed Section V.

II. BOUND STATES IN A QUANTUM WIRE

In this section we show the effect of the difference in the effective masses of the electron within the well and outside the well on the electron wave function for a single quantum well. Let the quantum wire with its length parallel to the z-axis be defined by the potentials

$V=-V_0$, for $|x|<a$ for all values of z and

$V=0$,for $|x|>a$, for all values of z

Since the system has the translational symmetry in the z direction the electron wave function in this direction is given by $\exp(ik_z z)$, where k_z can take any positive value. The wave function in the x-direction is obtained by solving the wave equations

$$-\frac{\hbar^2}{2m_a}\frac{\partial^2}{\partial x^2}\varphi(x)+\left[-V_o-E+\frac{\hbar^2}{2m_a}k_z^2\right]\varphi(x)=0 \quad \text{for } |x|<a \tag{2.1}$$

$$-\frac{\hbar^2}{2m_s}\frac{\partial^2}{\partial x^2}\varphi(x)+\left[-E+\frac{\hbar^2}{2m_s}k_z^2\right]\varphi(x)=0, \quad \text{for } |x|>a. \tag{2.2}$$

If the effective masses of the electron are the same so that $m_a=m_s=m$ for all values of x, the energy of the system will be simply given by

$$E=\frac{\hbar^2}{2m}k_z^2+E_n$$

where E_n are the eigenenergies of the electron bound to a potential well V_o. These energies and corresponding stationary states are given in standard textbooks on quantum mechanics . If the effective masses of the electron are different as assumed in writing the wave equations (2.1) and (2.2), then the wave functions and the eigenenergies of the system are dependent on the wave vector k_z. It is possible to express the effective potential V which is altered due the electronic motion in the z-direction according as

$$V= V_o+[\hbar^2k_z^2/2][(1/m_s)-(1/m_a)]. \tag{2.3}$$

As is clear from Eq. (2.3), when the effective masses are the same then the effect of the electronic motion in the z-direction on the electron wave function in the x-direction is removed.

The wave functions for the above system are

$$\varphi(x,z)=\begin{cases} Be^{k'x+ik_z z}, & \text{for } x<-(a/2); \\ A\cos(kx)e^{ik_z z}, & \text{for } |x|<(a/2); \\ Be^{-k'x+ik_z z}, & \text{for } x>(a/2); \end{cases} \tag{2.5}$$

where

$$k^2=[(2m_a/\hbar^2)(v_o+E)-k_z^2] \tag{2.6}$$

and

$$(k')^2=[k_z^2-(2m_sE/\hbar^2)]. \tag{2.7}$$

The boundary condition for the wave function produces the relation

$$\cot(ka/2)=\frac{[ka/2]}{\left[\frac{2m_sV_o(a/2)^2}{\hbar^2}-\frac{m_s}{m_a}(ka/2)^2+[1-(m_s/m_a)](k_za/2)^2\right]^{1/2}}. \tag{2.8}$$

Solving for (ka/2) in Eq.(2.8) and substituting the value in (2.6) gives the eigenenergy of the system for a prescribed value of k_z.

The normalization constants in (2.5) are given by:

$$B = A\cos(ka/2)e^{(k'a/2)}, \qquad (2.9)$$

where

$$A = [2/a]^{1/2}\left[\frac{\cos^2(ka/2)}{(k'a/2)} + 1 + \frac{\sin(ka)}{(ka)}\right]^{-(1/2)} . \qquad (2.10)$$

(See Appendix 1 for the full derivation of the result)

Since we are considering bound states for the electron in the x-direction, both k^2 and $(k')^2$ are positive. It therefore follows that

$$[\hbar^2 k_z^2/2m_s] > E > [(\hbar^2 k_z^2/2m_a) - V_o]. \qquad (2.11)$$

Figure 2 describes the system with the wave functions of the electron for various values of k_z. The wave function parellel to the wire is $e^{ik_z z}$ and is not shown in the figure.

III. PROBABILITY AMPLITUDES

Let the wave functions of the electron in well 1 and 2 be φ_1 and φ_2, respectively. These wave functions are obtained by considering each well in isolation. The wave functions are therefore uncoupled and they are not orthogonal to each other. The two wave functions would overlap and the overlap integral would be finite depending on the separating distance between the wells. We consider only bound states of the system and assume for simplicity that there are only two such states. It should be recognized that the these states are bound in the sense that the wave functions are restricted by the width of the well but they unrestricted in the direction along the length of the well.

We assume that the state Ψ of the electron in the presence of both the wires can be described in terms of the individual wave functions of the two wires. Clearly this is the assumption since the wave functions are not orthogonal. The assumption is quite frequently made in such calculations and is known to give reasonably reliable results. It therefore follows that:

$$\Psi(x,z,t)=\sum_{n} a_n\varphi_n, \tag{3.1}$$

where a_n's are time dependent coefficients and for our system n takes values 1 and 2. The amplitude of finding the electron in state φ_j is C_j and is given by

$$C_j=<\varphi_j|\Psi>, \tag{3.2}$$

If the wave functions φ_j's were orthogonal then $a_j=C_j$. The time dependence of the amplitude C_j is given by

$$\frac{\partial C_j}{\partial t}=<\varphi_j|\frac{\partial}{\partial t}|\Psi>. \tag{3.3}$$

The time dependence of the state Ψ is determined by

$$i\hbar\frac{\partial\Psi}{\partial t} = H\Psi, \tag{3.4}$$

where the Hamiltonian of the entire system consisting of both the quantum wires is included in H. If we now substitute (3.1) into (3.3) and (3.4) we get

$$\frac{\partial C_j}{\partial t} = \sum_n \frac{\partial a_n}{\partial t} \int \varphi_j^* \varphi_n dx \ , \tag{3.5}$$

and

$$i\hbar \frac{\partial}{\partial t} \sum_n a_n \varphi_n = \sum_n a_n H \varphi_n \tag{3.6}$$

We now multiply (3.6) by φ_j^* and integrate over the x variable and comparing the result with (3.5) we obtain

$$\frac{\partial}{\partial t} C_j = (1/i\hbar) \sum E_{jn} C_n , \tag{3.7}$$

where E_{ji} are defined by the relation

$$H \varphi_j^* = \sum_n E_{jn} \varphi_n^* . \tag{3.8}$$

For the two state system Eq. (3.7) can be written as

$$\frac{\partial}{\partial t} C_1=(1/ih)[E_{11}C_1+E_{12}C_2], \tag{3.9}$$

and

$$\frac{\partial}{\partial t} C_2=(1/ih)[E_{21}C_1+E_{22}C_2]. \tag{3.10}$$

Here the E's are obtained from the relation (3.8) which for two quantum states we get:

$$E_{11}=[\beta_{11}-\beta_{21}\alpha_{12}]/[1-\alpha_{21}\alpha_{12}];$$
$$E_{12}=[\beta_{11}\alpha_{21}-\beta_{21}]/[\alpha_{12}\alpha_{21}-1];$$
$$E_{21}=[\beta_{12}-\beta_{22}\alpha_{12}]/[1-\alpha_{12}\alpha_{21}];$$
$$E_{22}=[\beta_{12}\alpha_{21}-\beta_{22}]/[\alpha_{12}\alpha_{21}-1]. \tag{3.11}$$

where

$$\alpha_{ij}=\langle\varphi_i\varphi_j\rangle \text{ and } \beta_{ij}=\langle\varphi_i H\varphi_j\rangle. \tag{3.12}$$

If C's are assumed to have time dependence according as $\exp(-i\gamma t)$ then the secular equation giving the frequencies is given by

$$\begin{vmatrix} \hbar\gamma - E_{11} & E_{12} \\ E_{21} & \hbar\gamma - E_{22} \end{vmatrix} = 0 \qquad (3.13)$$

Solving Eq.(3.13) for γ get

$$2\hbar\gamma = [E_{11}+E_{22}] \pm [(E_{11}-E_{22})^2+4E_{12}E_{21}]^{1/2}. \qquad (3.14)$$

The probability amplitude C_1 is given by

$$C_1 = g\ \exp(-i\gamma_1 t) + h\ \exp(-i\gamma_2 t) \qquad (3.15)$$

where g and h are constants which are determined by initial boundary conditions. If we assume that the probability of finding the electron in state φ_1 at time t=0 is zero, then h=-g. C_1 is then given by

$$C_1 = g[\exp(-i\gamma_1 t) - \exp(-i\gamma_2 t)]$$

and

$$C_1C_1^*=4gg^*\sin^2[(\gamma_1-\gamma_2)t]. \tag{3.16}$$

Substituting for γ's, we get

$$C_1C_1^* =4gg^*\sin^2\omega t, \tag{3.17}$$

where the frequency of oscillations of the electron wave is given by ω according as

$$(\hbar\omega)^2= [(E_{11}-E_{22})^2+4E_{12}E_{21}]. \tag{3.18}$$

For symmetric quantum wells $E_{11}=E_{22}$, and the frequency of oscillations is then given by:

$$(\hbar\omega)^2=4E_{12}E_{21}. \tag{3.19}$$

IV. CALCULATION OF FREQUENCIES

The frequency of oscillations for the electron wave is given by Eq. (3.18) and (3.19). These depend on E's which in turn depend on α and β. To evaluate α's and β's we first write for φ_1 and φ_2 which are the wave functions for the electron in two uncoupled quantum wires. We consider the wires to be separated by distance $2L_0$ about the origin. For explanation see Fig. 2. The wave function φ_1 is obtained by transforming the origin by $L+(a/2)$ and φ_2 by $-L-(a/2)$ in the definition of φ given in Eq. (2.5). Thus

$$\varphi_1(x,z)= \varphi[x-(L+\{a/2\})], \tag{4.1}$$

and

$$\varphi_2(x,z)= \varphi[x+(L+\{a/2\})]. \tag{4.2}$$

Substituting (2.5) into (4.1),(4.2) and using the result in (3.10), we get

$$\alpha_{12}=(a/2)B^2 \frac{e^{-2(k'a/2)(\sigma+1)}}{(k'a/2)} + \sigma aB^2 e^{-(k'a)(\sigma+1)} + aABe^{-(k'a/2)(\sigma+1)} \text{ X } \left[\frac{e^{-\sigma(k'a/2)}}{(ka/2)^2+(k'a/2)^2} \text{ X } \left[(k'a/2)\cos(ka/2)[1-e^{(-k'a)}]+(ka/2)\sin(ka/2)[1+e^{k'a}]\right]\right], \tag{4.3}$$

where $\sigma=L_o/(a/2)$. $\alpha_{11}=\alpha_{22}=1$ by virtue of the normalization condition and $\alpha_{21}=\alpha_{12}$ by virtue of the symmetry of the system.

(See Appendix 2 for the derivation of the α results)

Following the same procedure used in obtaining α's, we now obtain β's.

We write β's in units of $[\hbar^2/2m_a(a/2)^2]$ to give:

$$\frac{\beta_{11}}{\left[\hbar^2/[2m_a(a/2)^2]\right]} = \gamma'^2\alpha_{11}+\left[(\epsilon-1)\gamma'^2-\gamma_o^2\right] \mathrm{X}$$

$$\frac{(a/2)B^2}{k'a} e^{-2(k'a)\sigma}\left[e^{-k'a}-e^{-3k'a}\right], \qquad (4.4)$$

and

$$\frac{\beta_{12}}{\left[\hbar^2/[2m_a(a/2)^2]\right]} = \gamma'^2\alpha_{12}+\left[(\epsilon-1)\gamma'^2-\gamma_o^2\right] \mathrm{X}$$

$$(a/2)BAe^{-(k'a/2)(2\sigma+1)}\left[\frac{[1+e^{k'a}]}{(ka/2)^2+(k'a/2)^2}\right] \mathrm{X}$$

$$\left[(k'a/2)\cos(ka/2)+(ka/2)\sin(ka/2)\right], \qquad (4.5)$$

By symmetry considerations $\beta_{11}=\beta_{22}$ and $\beta_{12}=\beta_{21}$. In Eqs. (4.4) and (4.5) we have used the following definitions:

$$\gamma_0^2 = V_0/[\hbar^2/2m_a(a/2)^2], \tag{4.6}$$

$$\gamma'^2 = (ka/2)^2 + (k_z a/2)^2 - \gamma_0^2, \tag{4.7}$$

$$\epsilon = (m_s/m_a), \tag{4.8}$$

and in terms of ϵ, k'^2 is (using Eqs. (2.6) and (2.7)) given by

$$(k'a/2)^2 = (k_z a/2)^2 - \epsilon\gamma'^2. \tag{4.9}$$

(See Appendix 3 for the derivation of the β results)

V. WAVE PACKET FORMULATION

Recall that we have made the assumption that the wave function for the two well system is a linear combination of the individual wells' wave functions (see equation (3.1)). Since the φ's are not orthogonal, $\langle\varphi_1|\varphi_2\rangle$ is not zero. Also, $a_1 a_1^*$ from equation (3.1) is not the probability of finding the electron in state φ_1 neither do the wave functions φ form a complete set.

Having made the assumption that the system may be represented by a linear combination we note that the probability of finding the electron in state φ_j is $C_j C_j^*$ where C_j is given by equation (3.2) or

$$C_j = \int \psi(r,t)\varphi_j^*(r) d^3r = \int \sum_l a_l \varphi_l \varphi_n^* d^3r = \sum_l a_l \int \varphi_l \varphi_n^* d^3r \qquad \ldots(5.1)$$

Thus, for two wells,

$$C_1 = a_1\alpha_{11} + a_2\alpha_{12} \quad \text{and} \quad C_2 = a_1\alpha_{21} + a_2\alpha_{22} \qquad \ldots(5.2)$$

which leads to:

$$a_1 = [C_1\alpha_{22} - C_2\alpha_{12}] \;/\; [\alpha_{11}\alpha_{22} - \alpha_{21}\alpha_{12}]$$

$$a_2 = [C_1\alpha_{21} - C_2\alpha_{11}] \;/\; [\alpha_{21}\alpha_{12} - \alpha_{11}\alpha_{22}] \qquad \ldots(5.3).$$

Now, we recall (3.15) and write C_2 also (with the minor modification that the constants 'g' and 'h' from (3.15) are now

'g_1' and 'h_1'):

$$C_1 = g_1 \exp(-i\gamma_1 t) + h_1 \exp(-i\gamma_2 t)$$

$$C_2 = g_2 \exp(-i\gamma_1 t) + h_2 \exp(-i\gamma_2 t) \qquad \ldots(5.4).$$

One possible solution is arrived at utilizing the choice of $g_1 = g_2$ and $h_2 = -h_1$. From $\Psi = a_1\varphi_1 + a_2\varphi_2$ we then arrive at

$$\Psi = \left[\exp(-i\gamma_1 t) g_1 [1+\alpha_{12}][\varphi_1+\varphi_2] + \exp(-i\gamma_2 t) h_1 [1-\alpha_{12}][\varphi_1-\varphi_2]\right] \qquad \ldots(5.5).$$

Further, any arbitrary wave function can now be expressed as:

$$\Psi = \sum_{k_z} A_{k_z} \frac{[\varphi_1+\varphi_2]\exp(-i\gamma_1 t+ik_z z)}{[2(1+\alpha_{12})]^{1/2}} + \sum_{k_z} B_{k_z} \frac{[\varphi_1-\varphi_2]\exp(-i\gamma_2 t+ik_z z)}{[2(1-\alpha_{12})]^{1/2}} \qquad \ldots(5.6).$$

The choice of wave packet desired is the Gaussian which has

$$\Psi_{t=0} = \varphi_1 \exp(-\xi z^2/2 + ik_{zo} z) \qquad \ldots(5.7).$$

The constants A_{k_z} and B_{k_z} are as yet unknown. They may be found by multiplying the right hand side of (5.6) (at t = 0) by $\exp(-ik_z'z)\cdot[\varphi_1+\varphi_2]/[2(1+\alpha_{12})]^{1/2}$ and integrating over x and k_z to reduce the whole right hand side to $A_{k_z'}$, which is then obviously equal to:

$$A_{k_z} = \int \varphi_1 \exp[\xi z^2/2 + i(k_{zo}-k_z')z][\varphi_1+\varphi_2]/[2(1+\alpha_{12})]^{1/2} dx dk_z$$

and similarly

$$B_{k_z} = \int \varphi_1 \exp[\xi z^2/2 + i(k_{zo}-k_z')z][\varphi_1-\varphi_2]/[2(1-\alpha_{12})]^{1/2} dx dk_z .$$

These two can now be substituted back into (5.6) to give the wave packet at any time t.

The group velocity for the wave packet is then simply

$$V_{g_1} = \left[\frac{\delta\gamma_1}{\delta k_z}\right]_{k_z=k_{zo}} , \quad V_{g_2} = \left[\frac{\delta\gamma_2}{\delta k_z}\right]_{k_z=k_{zo}}$$

VI. NUMERICAL RESULTS

In this section we evaluate the frequencies of the electron oscillating between the two quantum wires using Eq. (3.19). Our procedure is as follows: We fix values of ϵ and γ_0^2 and use (a/2) as the unit of length where (a) is the width of the quantum well. For the present numerical calculations we consider $\epsilon=1.37$ and $\epsilon\gamma_0^2=3.00$, which are reasonable values[4] for a GaAs-AlGaAs system. We treat the $k_z a/2$ as a parameter which measures the speed of the electron wave parallel to the quantum wire. We obtain the value (ka/2) by solving the transcendental equation (2.8). We then fix the values of γ'^2 using (4.7) and $(k'a/2)^2$ using (4.9). The normalization constants A and B are obtained from equations (2.9) and (2.10). The numerical values for α's and β's are derived using eqns. (4.3)-(4.5). E's are determined with the help of (3.11) and finally the oscillatory frequency is derived from eqn. (3.19).

In figure 2 we have shown normalized wave functions for the ground state of an electron in a single quantum wire in which the electron motion is determined by a potential well of depth $-V_0$ and width (a) in the x-direction and constant potential along the length of the wire. The wave functions are shown for the x-direction using (a/2) as the unit of length. The wave functions are affected by the electronic motion in the z-direction. The normalized wave functions are shown for values $(k_z a/2) = 0$, 1.00, and 2.00. We observe that as the value of $k_z a/2$ increases, the effective depth of the potential decreases leading to increased spread of the wave function outside the well. For a two wire system the spread leads to greater overlap between the wave functions and an increased value for the frequency of the electron oscillations between the two wires.

In figure 3 we have shown the variation of the oscillatory frequency of the electron as a function of the distance separating the two quantum wires. The frequency is large for small separations but as the distance increases the frequency falls rapidly. The variations are shown for three values of $k_z a/2$ and, as expected, as $k_z a/2$ increases the frequency of oscillations also increases.

In figure 4, we have shown the variation of frequency as a function of the depth of the potential of the well. As the depth increases the electron wave function becomes increasingly confined. The overlap of the wavefunctions between the two wells decreases and so also the oscillatory frequency of the electron.

In figure 5, we have shown the variation of group velocity as a function of $k_z a/2$. As the value of the z-direction wave number multiplied by the well half-width increases, the wave packet group velocity increases in magnitude. It may be noted that the wavefunction group velocities, V_{g_1} and V_{g_2}, diverge in value as $k_z a/2$ grows large.

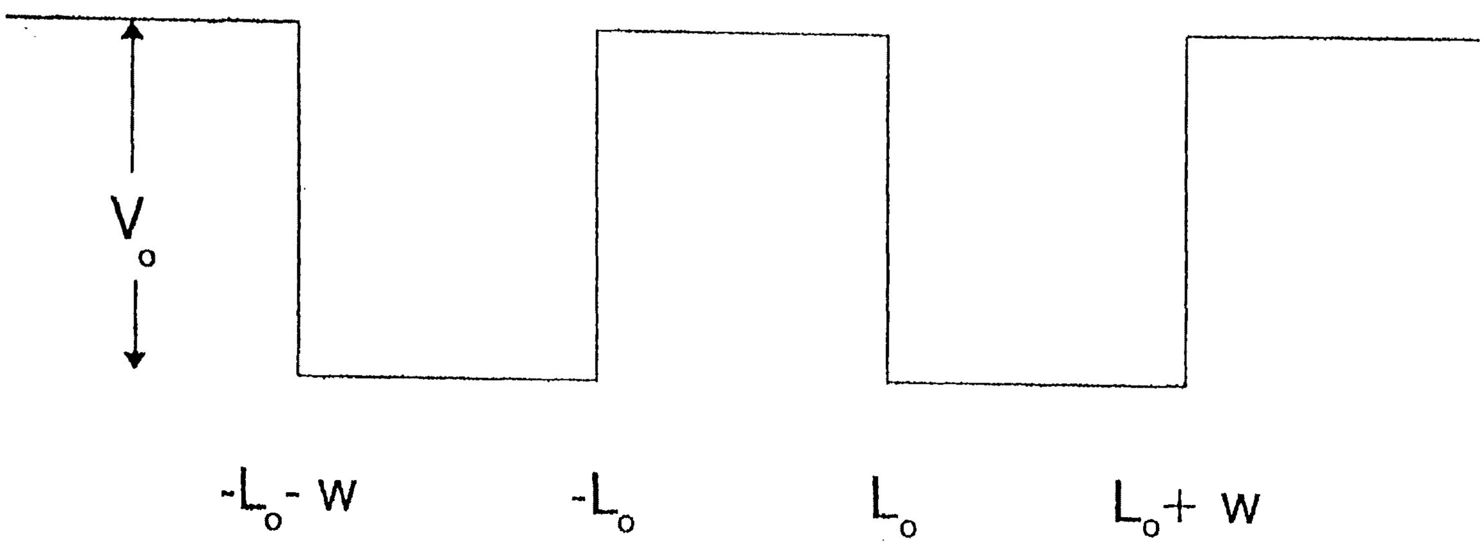


Fig.1: The variation of potential in the direction normal to the length of the wires.

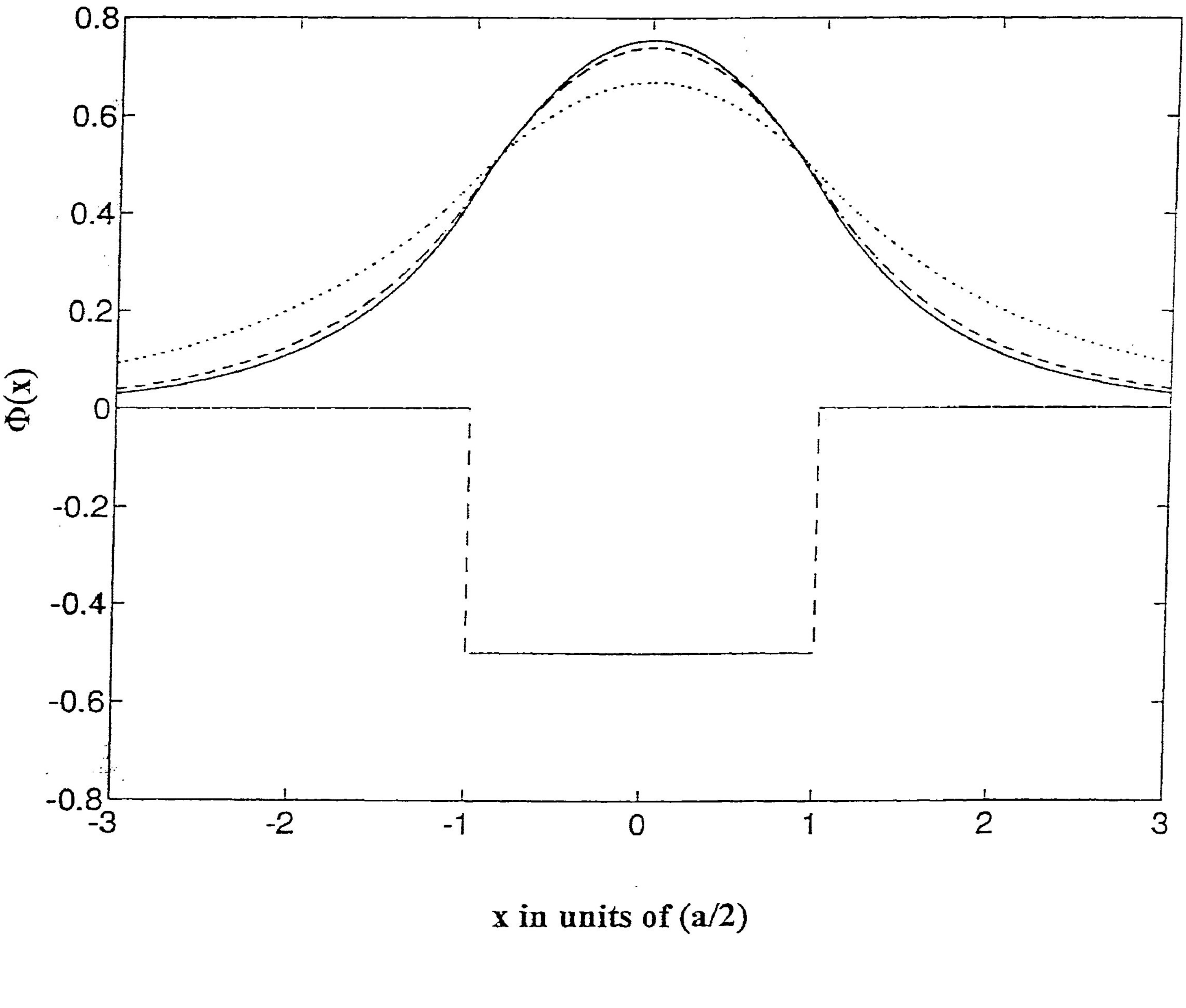


Fig.2: The wave functions of a finite potential well as a function of distance measured in units of (a/2). The continuous, dashed and dotted curves are for $k_z a/2$ equal to 0, 1 and 2 respectively.

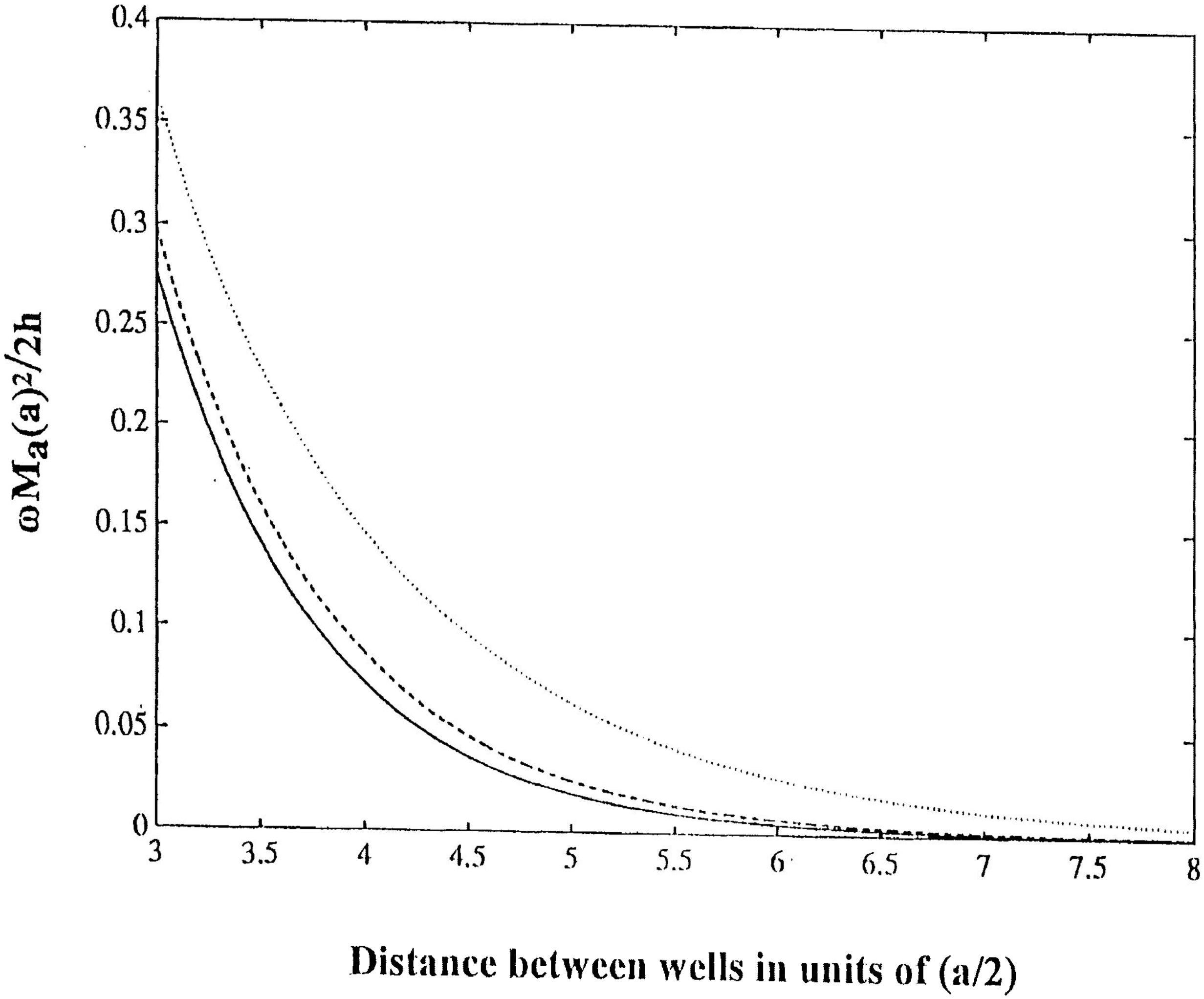
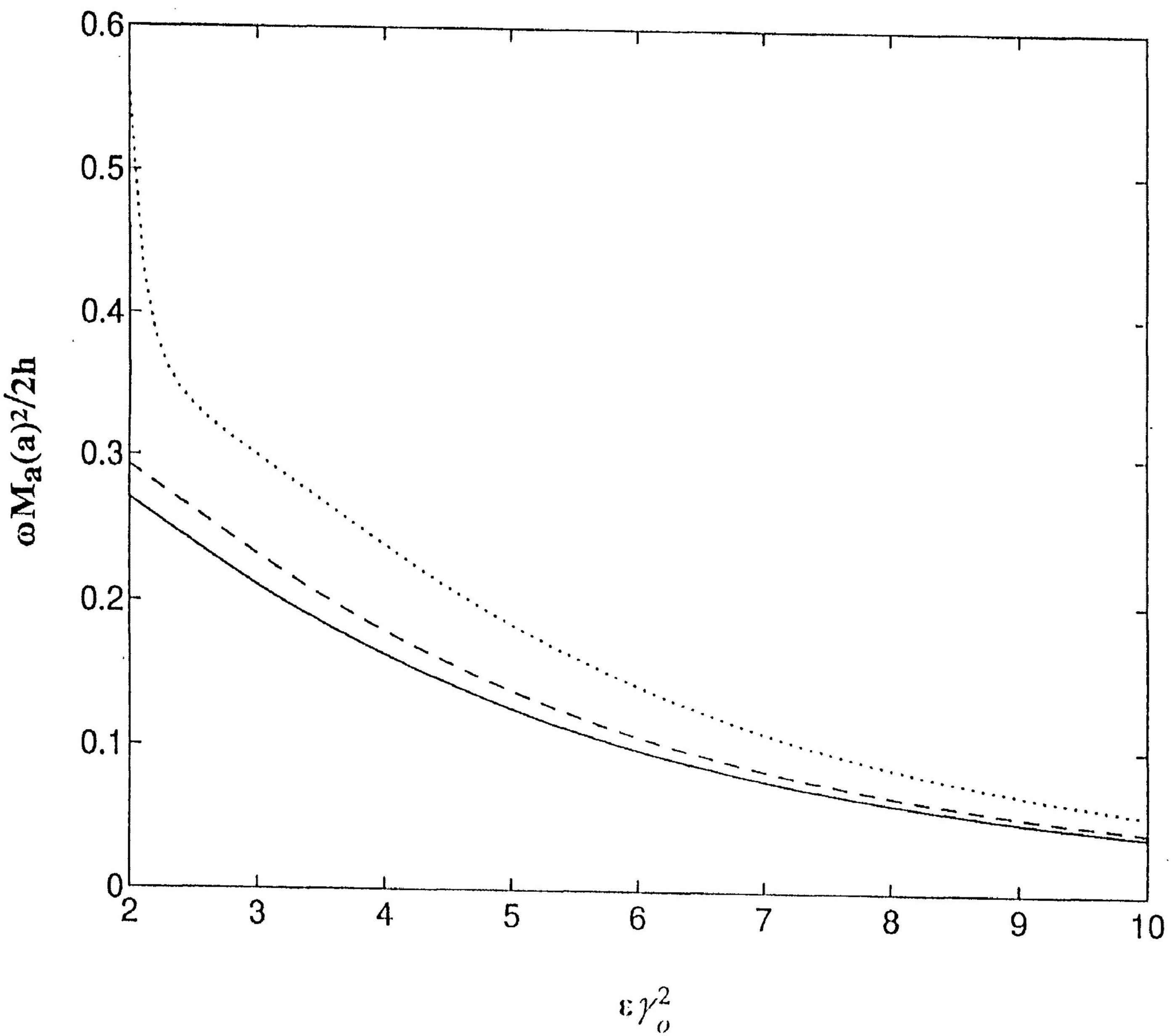


Fig.3: The frequency of oscillations of an electron wave in units of $(2\hbar^2/m_a a^2)$ as a function of the distance separating the wires in units (a/2). The continuous, dashed and doted curves are for $k_z a/2$

Fig.4: The frequency of oscillations of an electron wave in units of $(2\hbar^2/m_a a^2)$ as a function of $\epsilon\gamma_0^2$. The continuous, dashed and dotted curves are for $k_z a/2$ equal to 0, 1 and 2 respectively.



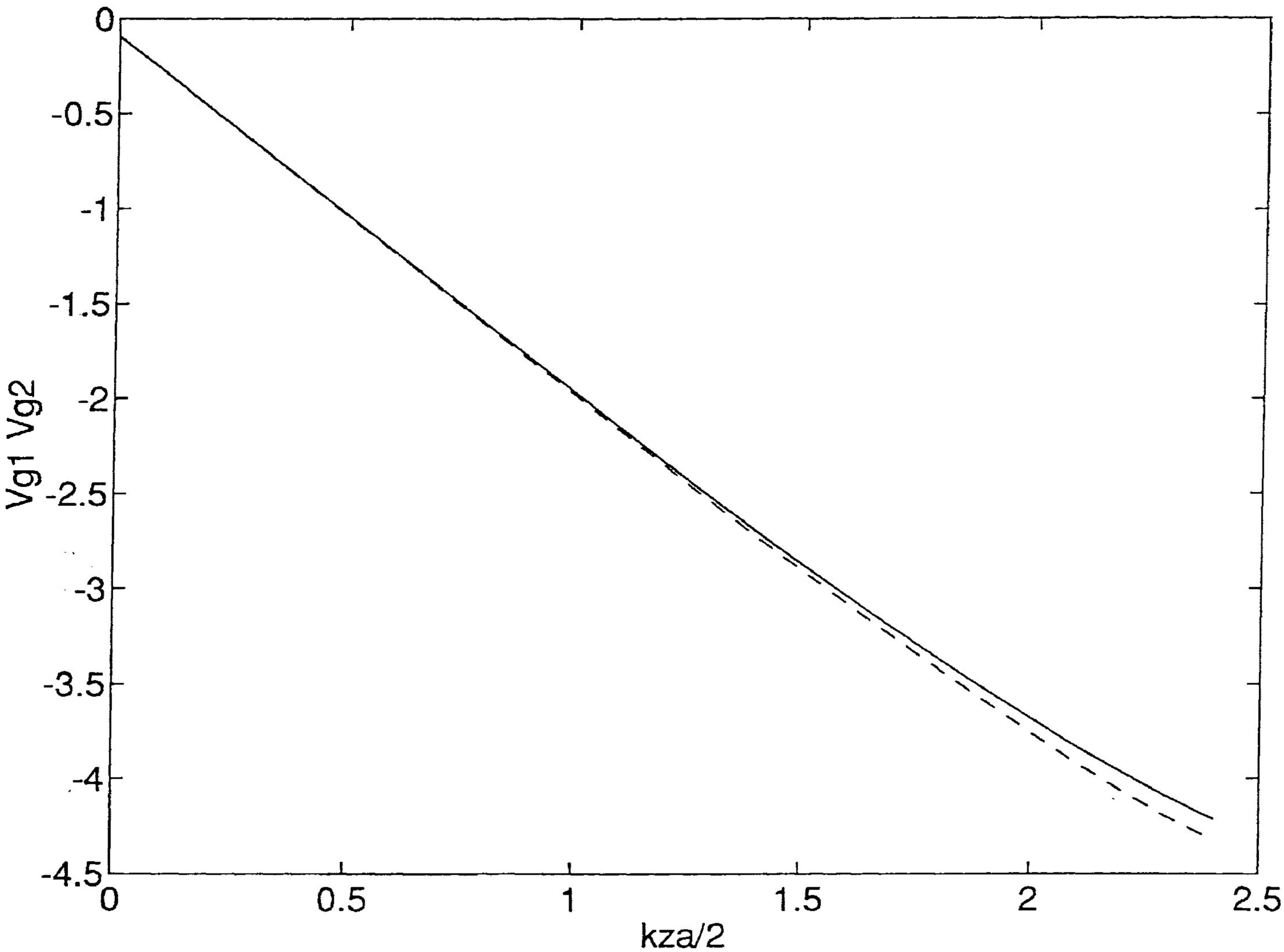


Fig.5: The group velocities V_{g_1} and V_{g_2} of the wave packets from section V. as a function of the value $k_z a/2$. The continuous line represents V_{g_1} and the dashed line V_{g_2}.

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Appendix 1: Bound States

We begin by considering a quantum well in two dimensions which we call x and z.

Consider the Schrödinger equation in the region outside the well:

$$-\frac{\hbar^2}{2m_s}\left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial z^2}\right]\varphi(x,z,t) = i\hbar\frac{\partial}{\partial t}\varphi(x,z,t) \qquad \ldots. (1.1)$$

This may be solved using:

$$\varphi(x,z,t) = A_t e^{-iEt}\phi(x)\phi(z)$$

which results in equation 1.1 becoming :

$$-\frac{\hbar^2}{2m_s}\left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial z^2}\right]\phi(x)\phi(z) = E\phi(x)\phi(z) \qquad \ldots. (1.2)$$

Multiplying equation 1.2 by:

$$\frac{-2m_s}{\hbar^2\phi(x)\phi(z)}$$

gives:

$$\frac{1}{\phi(x)}\frac{\partial^2}{\partial x^2}\phi(x) + \frac{1}{\phi(z)}\frac{\partial^2}{\partial z^2}\phi(z) = -\frac{2m_sE}{\hbar^2}$$

which allows for separation of the x and z parts which we do in the following manner arbitrarily (but with purpose):

$$\frac{1}{\phi(x)}\frac{\partial^2}{\partial x^2}\phi(x) + \frac{2m_sE}{\hbar^2} = -\frac{1}{\phi(z)}\frac{\partial^2}{\partial z^2}\phi(z) = k_{z1}^2 \qquad \ldots.(1.3)$$

The z component thus has the form:

$$\frac{\partial^2}{\partial z^2}\phi(z) + k_{z1}^2\phi(z) = 0$$

Now, k_{z1}^2 must be positive to avoid exploding wavefunctions as z goes to infinity, therefore:

$$\phi(z) = A_{z1}e^{\pm ik_{z1}z}$$

where k_{z1} takes positive and negative values.

Further, from 1.3,

$$\frac{1}{\phi(x)}\frac{\partial^2}{\partial x^2}\phi(x) + \frac{2m_sE}{\hbar^2} = k_{z1}^2$$

which leads to:

$$\frac{\partial^2}{\partial x^2}\phi(x) - \left[k_{z1}^2 - \frac{2m_sE}{\hbar^2}\right]\phi(x) = 0$$

which has solutions

$$\phi(x) = \begin{cases} A_x e^{-k'x} & \text{for } x > a/2 \\ A_x e^{k'x} & \text{for } x \leq a/2 \end{cases}$$

where $k'^2 = \left[k_{z1}^2 - 2m_sE/\hbar^2\right]$.

Now, we have chosen to consider a solution localized within the well and decaying outside the well. Such a choice requires that k'^2 be positive. As k_{z1}^2 is also positive (as shown above) this leads to:

$$\left[k_{z1}^2 - 2m_sE/\hbar^2\right] > 0 \quad \text{or} \quad E < \frac{\hbar^2k_{z1}^2}{2m_s}$$

which means that E can have all negative values and *can* have positive values. The E values will, of course, be determined by the boundary conditions.

Inside the Well

Inside the well there is an added potential term in the Schrödinger equation:

$$-\frac{\hbar^2}{2m_a}\left[\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial z^2}\right]\varphi(x,z,t) - V_o\varphi(x,z,t) = i\hbar\frac{\partial}{\partial t}\varphi(x,z,t)$$

Again, assuming a solution

$$\varphi(x,z,t) = A_t e^{-iEt}\phi(x)\phi(z)$$

leads to a time-independent equation in x and z:

$$-\frac{\hbar^2}{2m_a}\left[\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial z^2}\right]\phi(x)\phi(z) - V_o\phi(x)\phi(z) = E\phi(x)\phi(z)$$

multiplying by

$$\frac{-2m_a}{\hbar^2\phi(x)\phi(z)}$$

yields

$$\frac{1}{\phi(x)}\frac{\partial^2}{\partial x^2}\phi(x) + \frac{1}{\phi(z)}\frac{\partial^2}{\partial z^2}\phi(z) + \frac{2m_s}{\hbar^2}(V_o + E) = 0$$

As before, one can set the components of the equation equal to some constant:

$$\frac{1}{\phi(x)}\frac{\partial^2}{\partial x^2}\phi(x) + \frac{2m_s}{\hbar^2}(V_o + E) = -\frac{1}{\phi(z)}\frac{\partial^2}{\partial z^2}\phi(z) = k_{z2}^2$$

and thus

$$\frac{\partial^2}{\partial z^2}\phi(z) + k_{z2}^2\phi(z) = 0$$

which leads to

$$\phi(z) = A_{z2}e^{\pm ik_{z2}z}$$

as k_{z2}^2 must be positive to avoid exploding wave functions as z goes to infinity and k_{z2} can take positive or negative values.

Further,

$$\frac{1}{\phi(x)}\frac{\partial^2}{\partial x^2}\phi(x) + \frac{2m_a}{\hbar^2}(V_\circ + E) - k_{z2}^2 = 0$$

or

$$\frac{\partial^2}{\partial x^2}\phi(x) + \left[\frac{2m_a}{\hbar^2}(V_\circ + E) - k_{z2}^2\right]\phi(x) = 0$$

which has the solution (for lowest E):

$$\phi(x) = A_{x2}\cos kx$$

where

$$k^2 = \left[\frac{2m_a}{\hbar^2}(V_\circ + E) - k_{z2}^2\right]$$

Now, we are still considering a solution localized within the well and decaying outside the well and this requires k^2 be positive. Also, we know that k_{z2}^2 must also be positve. Thus,

$$\left[E + V_\circ - \frac{\hbar^2 k_{z2}^2}{2m_a}\right] > 0 \quad \text{or} \quad E > \left[-V_\circ + \frac{\hbar^2 k_{z2}^2}{2m_a}\right]$$

and using the inequality from outside the well,

$$\left[\frac{\hbar^2 k_{z1}^2}{2m_s}\right] > E > \left[\frac{\hbar^2 k_{z2}^2}{2m_a} - V_\circ\right]$$

Matching $\phi(z)$ leads to $A_{z1}=A_{z2}$ and $k_{z1}=k_{z2}$. Henceforward, the combined $\phi(x)$, $\phi(z)$ coefficients will be denoted A, and B. Therefore:

$$\varphi(x,z) = \begin{cases} A\cos kx \bullet e^{ik_z z} & \ldots.\ -a/2 < x < a/2 \\ Be^{k'x} \bullet e^{ik_z z} & \ldots.\ x < -a/2 \\ Be^{-k'x} \bullet e^{ik_z z} & \ldots.\ x > a/2 \end{cases}$$

Deriving the implicit equation for finding ka/2

The boundary conditions are now used to find an implicit equation with which we can find ka/2.

At $x = a/2$,

$$A\cos(ka/2) = Be^{-k'a/2} \qquad \ldots..\ (1.4)$$

(d/dx of eqn 4)
$$-Ak\sin(ka/2) = -k'Be^{-k'a/2} \qquad \ldots..\ (1.5)$$

(eqn 4/eqn 5)
$$\frac{1}{-k}\cot(ka/2) = \frac{1}{-k'} \qquad \ldots..\ (1.6)$$

Further, equation 1.6 can be rearranged like so:

$$\cot(ka/2) = \frac{k}{k'} \quad \text{or} \quad \cot(ka/2) = \frac{k}{\left[k_z^2 - \frac{2m_s E}{\hbar^2}\right]^{(1/2)}}$$

and recalling that

$$k^2 = \frac{2m_a}{\hbar^2}(V_\circ + E) - k_z^2 \quad \text{or} \quad E = \left[\, k^2 + k_z^2 \,\right]\frac{\hbar^2}{2m_a} - V_\circ$$

we arrive at

$$\cot(ka/2) = \frac{k}{\left[k_z^2 - \frac{2m_s}{\hbar^2}\left[\frac{\hbar^2}{2m_a}\left[k^2+k_z^2\right]-V_o\right]\right]^{(1/2)}}$$

$$\rightarrow\cot(ka/2) = \frac{k}{\left[k_z^2 - \frac{m_s}{m_a}k^2 - \frac{m_s}{m_a}k_z^2 + \frac{2m_sV_o}{\hbar^2}\right]^{(1/2)}} \quad \ldots. (1.7) .$$

To achieve our goal of an implicit equation to solve for ka/2 we simply multiply equation 1.7 by (a/2)/(a/2) - ie 1 - on the RHS:

$$\cot(ka/2) = \frac{(ka/2)}{\left[\frac{2m_sV_o(a/2)^2}{\hbar^2} - \frac{m_s}{m_a}(ka/2)^2 + \left[1 - \frac{m_s}{m_a}\right]\left[k_za/2\right]^2\right]^{(1/2)}} \quad \ldots(1.8)$$

Equation 1.8 is solved by plotting the right hand side of the equation and also the left and determining the intercepts - ie solutions. This is done by computer.

Normalization Constants

The wave function coefficients A and B are found through normalization of the wave function. Again at x = a/2:

$$A\cos(ka/2) = Be^{-k'a/2} \qquad \text{or} \qquad B = \frac{A\cos(ka/2)}{e^{-k'a/2}}$$

The normalization condition states $\int_{-\infty}^{+\infty}\psi^*\psi dx = 1$. In our case this results in:

$$\int_{-\infty}^{-a/2} Be^{k'x}Be^{k'x}dx + \int_{-a/2}^{+a/2} A^2\cos^2(kx)dx + \int_{a/2}^{+\infty} B^2e^{-2k'x}dx = 1$$

Now,

$$\int_{-\infty}^{-a/2} B^2 e^{k'x} dx = \int_{a/2}^{+\infty} B^2 e^{-k'x} dx = A^2 \left[\frac{\cos^2(ka/2)}{2k'} \right]$$

and,

$$\int_{-a/2}^{+a/2} A^2 \cos^2(kx) dx = \frac{A^2}{2} \int_{-a/2}^{+a/2} \left[\cos(2kx) + 1 \right] dx = \frac{A^2}{2} \left[\frac{2}{2k} \sin(2ka/2) + a \right]$$

thus:

$$A^2 \left[\frac{\cos^2(ka/2)}{2k'} \right] + A^2 \left[\frac{1}{2k} \sin(2ka/2) + \frac{a}{2} \right] + A^2 \left[\frac{\cos^2(ka/2)}{2k'} \right] = 1 \qquad \ldots (1.9)$$

We must now solve for A realizing that we would prefer not to have to fix k and k' - ie we would prefer to solve for A with an equation that is in terms of ka/2 and k'a/2, which we have just solved for (k'a/2 is just the denominator in equation 8 - once we have ka/2, k'a/2 is easily calculated). To do this we multiply A by $\sqrt{a/2}$. From equation 9:

$$A = \frac{1}{\left[\frac{\cos^2(ka/2)}{k'} + \frac{a}{2} + \frac{\sin(2ka/2)}{2k} \right]^{(1/2)}}$$

$$\Rightarrow \sqrt{a/2}\, A = \frac{1}{\left[\frac{\cos^2(ka/2)}{k'a/2} + 1 + \frac{\sin(2ka/2)}{2ka/2} \right]^{(1/2)}}$$

Appendix 2: Alpha Values

In section III we defined α as $\alpha_{ij} = \langle\varphi_i|\varphi_j\rangle$. Thus,

$\alpha_{11} = \langle\varphi_1|\varphi_1\rangle = 1$

$\alpha_{22} = \langle\varphi_2|\varphi_2\rangle = 1$

and $\alpha_{12} = \langle\varphi_1|\varphi_2\rangle = \int_{-\infty}^{+\infty} \phi_1(x)\phi_2(x)dx$

since ψ_1 and ψ_2 are identical and symmetrically distanced from the zero point of the x-axis (thus $\phi_1^*(z)\bullet\phi_2(z) = 1$ and periodic boundary conditions can be used to remove the z dependence of α_{12}). As this is the case, $\alpha_{12} = \alpha_{21}$ (as neither $\phi_1(x)$ or $\phi_2(x)$ is complex). Now,

$$\int_{-\infty}^{+\infty} \phi_1(x)\phi_2(x)dx = \int_{-\infty}^{-(L_o+a)} Be^{k'(x+L_o+a/2)}\bullet Be^{k'(x-L_o-a/2)}dx \quad \ldots \text{ I}$$

$$+$$

$$\int_{-(L_o+a)}^{-L_o} A\cos[k(x+L_o+a/2)]\bullet Be^{k'(x-L_o-a/2)}dx \quad \ldots \text{ II}$$

$$+$$

$$\int_{-L_o}^{+L_o} Be^{-k'(x+L_o+a/2)}\bullet Be^{k'(x-L_o-a/2)}dx \quad \ldots \text{ III}$$

$$+$$

$$\int_{L_o}^{L_o+a} Be^{-k'(x+L_o+a/2)}A\cos[k(x-L_o-a/2)]dx \quad \ldots \text{ IV}$$

$$+$$

$$\int_{L_o+a}^{+\infty} Be^{-k'(x+L_o+a/2)}\bullet Be^{-k'(x-L_o-a/2)}dx \quad \ldots \text{ V}$$

These integrals are solved region by region as follows:

$$I \rightarrow \int_{-\infty}^{-(L_o+a)} Be^{k'(x+L_o+a/2)} \bullet Be^{k'(x-L_o-a/2)} dx$$

$$= B^2 \int_{-\infty}^{-(L_o+a)} e^{2k'x} dx$$

$$= B^2 \left[\frac{e^{2k'(-L_o-a)} - e^{2k'(-\infty)}}{2k'} \right]$$

$$= B^2 \left[\frac{e^{-2k'(L_o+a)}}{2k'} \right]$$

$$II \rightarrow \int_{-(L_o+a)}^{-L_o} A\cos[k(x+L_o+a/2)] \bullet Be^{k'(x-L_o-a/2)} dx$$

$$= ABe^{-k'(L_o+a/2)} \int_{-(L_o+a)}^{-L_o} \cos[k(x+L_o+a/2)] e^{k'x} dx$$

$$= ABe^{-k'(L_o+a/2)} \left[\frac{e^{k'x}}{k^2+(-k')^2} \left[k'\cos[k(x+L_o+a/2)] + \sin[k(x+L_o+a/2)] \right] \right]_{-(L_o+a)}^{-L_o}$$

$$= ABe^{-k'(L_o+a/2)} \left[\frac{e^{-k'L_o}}{k^2+k'^2} \left[k'\cos(ka/2) + k\sin(ka/2) \right] - \frac{e^{-k'(L_o+a)}}{k^2+k'^2} \left[k'\cos(-ka/2) + k\sin(-a/2) \right] \right]$$

$$= ABe^{-k'(L_o+a/2)} \left[\frac{e^{-k'L_o}}{k^2+k'^2} \left[k'\cos(ka/2) + k\sin(ka/2) - \right. \right.$$

$$e^{-k'a}k'\cos(ka/2) + e^{-k'a}k\sin(ka/2)\Big]\Big]$$

$$III \rightarrow \int_{-L_o}^{+L_o} Be^{-k'(x+L_o+a/2)} \bullet Be^{k'(x-L_o-a/2)}dx$$

$$= B^2e^{-2k'(L_o+a/2)}\int_{-L_o}^{+L_o} e^0 dx$$

$$= B^2e^{-2k'(L_o+a/2)}\Big[L_o-(-L_o)\Big]$$

$$= 2L_oB^2e^{-2k'(L_o+a/2)}$$

IV = II by symmetry considerations

V = I by symmetry considerations

Therefore,

$\alpha_{12} = \alpha_{21} = I + II + III + IV + V$

$$= \frac{B^2e^{-2k'(L_o+a)}}{k'} + 2L_oB^2e^{-2k'(L_o+a/2)} +$$

$$2ABe^{-k'(L_o+a/2)}\left[\frac{e^{-k'L_o}}{k^2+k'^2}\Big[k'[\cos(ka/2)][1-e^{-k'a}]\right.$$

$$\left. + k[\sin(ka/2)][1+e^{-k'a}]\Big]\right].$$

To make α dimensionless, multiply appropriately by a/2 and recall that $\sigma = L_o/(a/2)$. This leads to the following:

$$\alpha_{12}=\alpha_{21}=\frac{(a/2)B^2e^{-2(k'a/2)(\sigma+1)}}{k'a/2} + 2\sigma(a/2)B^2e^{-2(k'a/2)(\sigma+1)} +$$

$$2(a/2)ABe^{-(k'a/2)(\sigma+1)}\left[\frac{e^{-\sigma(k'a/2)}}{(ka/2)^2+(k'a/2)^2}\left[(k'a/2)[\cos(ka/2)][1-e^{-2k'a/2}]\right.\right.$$

$$\left.\left.+ (ka/2)[\sin(ka/2)][1+e^{-2k'a/2}]\right]\right]$$

Appendix 3: Beta Values

Unlike the α_{11} (α_{22}) value, β_{11} (β_{22}) does not reduce simply. This is because the Hamiltonian in the definition of β is a linear combination of the Hamiltonians for the individual wells. So,

$$\beta_{11} = \langle\varphi_1^*|H|\varphi_1\rangle = \int_{-\infty}^{+\infty} \varphi_1^* H \varphi_1 \, dxdz$$

$$\Rightarrow \beta_{11} = \int_{-\infty}^{+\infty} \phi_1(x)^* \left\{ \frac{-\hbar^2}{2m}\left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial z^2}\right] - V_o f \right\} \phi_1(x) \, dx$$

where, $m = (m_a - m_s)f + m_s$ and $f = \begin{cases} 1 \text{ inside the wells} \\ 0 \text{ outside the wells} \end{cases}$

Thus,

$$\beta_{11} = \int_{-\infty}^{-(L_o+a)} \phi_1^*(x) \left\{ \frac{-\hbar^2}{2m_s}\left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial z^2}\right] \right\} \phi_1(x) \, dx$$

$$+ \int_{-(L_o+a)}^{-L_o} \phi_1^*(x) \left\{ \frac{-\hbar^2}{2m_a}\left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial z^2}\right] - V_o \right\} \phi_1(x) \, dx$$

$$+ \int_{-L_o}^{+L_o} \phi_1^*(x) \left\{ \frac{-\hbar^2}{2m_s}\left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial z^2}\right] \right\} \phi_1(x) \, dx$$

$$+ \int_{+L_o}^{+(L_o+a)} \phi_1^*(x) \left\{ \frac{-\hbar^2}{2m_a}\left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial z^2}\right] - V_o \right\} \phi_1(x) \, dx$$

$$+ \int_{+(L_o+a)}^{+\infty} \phi_1^*(x) \left\{ \frac{-\hbar^2}{2m_s}\left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial z^2}\right] \right\} \phi_1(x) \, dx$$

$$\Rightarrow \beta_{11} = E_1\int_{-\infty}^{+\infty}\phi_1^*(x)\phi_1(x)dx + \left\{\left[\frac{m_s}{m_a} - 1\right]E_1 - V_\circ\right\}\int_{L_\circ}^{(L_\circ+a)}\phi_1^*(x)\phi_1(x)dx$$

$$= E_1\alpha_{11} + \left\{\left[\frac{m_s}{m_a} - 1\right]E_1 - V_\circ\right\}\int_{L_\circ}^{(L_\circ+a)}\phi_1^*(x)\phi_1(x)dx$$

Now we will make β a dimensionless quantity and equal to calculable quantities:

$$\frac{\beta_{11}}{\left[\hbar^2/\left[2m_a(a/2)^2\right]\right]} = \frac{2m_aE_1(a/2)^2}{\hbar^2} + \left[\left[\frac{m_s}{m_a} - 1\right]\frac{2m_aE_1(a/2)^2}{\hbar^2} - \frac{2m_aV_\circ(a/2)^2}{\hbar^2}\right]\int_{L_\circ}^{(L_\circ+a)}\phi_1^*(x)\phi_1(x)dx$$

$$= \gamma_1'^2 + \left[(\epsilon-1)\gamma_1'^2 - \gamma_\circ^2\right]\int_{L_\circ}^{(L_\circ+a)}B^2e^{-2k'(x+L_\circ+a/2)}dx$$

$$= \gamma_1'^2 + \left[(\epsilon-1)\gamma_1'^2 - \gamma_\circ^2\right]B^2\left[\frac{e^{-k'(2L_\circ+3a/2)}-e^{-2k'(2L_\circ+a/2)}}{-2k'}\right]$$

$$= \gamma_1'^2 + \left[(\epsilon-1)\gamma_1'^2 - \gamma_\circ^2\right]\frac{(a/2)B^2}{2(k'a/2)}\left[e^{-4k'L_\circ}\left[e^{-k'a} - e^{-3k'a}\right]\right]$$

and recalling $\sigma = L_\circ/(a/2)$, $\dfrac{\beta_{11}}{\left[\hbar^2/\left[2m_a(a/2)^2\right]\right]}$

$$= \gamma_1'^2 + \left[(\epsilon-1)\gamma_1'^2 - \gamma_\circ^2\right]\frac{(a/2)B^2}{2(k'a/2)}\left[e^{-4(k'a/2)\sigma}\left[e^{-2k'a/2} - e^{-6k'a/2}\right]\right]$$

$$= \frac{\beta_{22}}{\left[\hbar^2/\left[2m_a(a/2)^2\right]\right]}$$ via symmetry considerations (and noting that for the case of the double symmetric wells, $\gamma_1'^2 = \gamma_2'^2$).

$$\beta_{12} = \langle\varphi_1^*|H|\varphi_2\rangle = \int_{-\infty}^{+\infty} \varphi_1^* H\varphi_2 dxdz$$

$$\Rightarrow \beta_{12} = \int_{-\infty}^{+\infty} \phi_1(x)^* \left\{\frac{-\hbar^2}{2m}\left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial z^2}\right] - V_o f\right\}\phi_2(x)\ dx$$

where, $m = (m_a - m_s)f + m_s$ and $f = \begin{cases} 1 \text{ inside the wells} \\ 0 \text{ outside the wells} \end{cases}$

Thus,

$$\beta_{12} = \int_{-\infty}^{-(L_o+a)} \phi_1^*(x)\left\{\frac{-\hbar^2}{2m_s}\left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial z^2}\right]\right\}\phi_2(x)\ dx$$

$$+ \int_{-(L_o+a)}^{-L_o} \phi_1^*(x)\left\{\frac{-\hbar^2}{2m_a}\left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial z^2}\right] - V_o\right\}\phi_2(x)\ dx$$

$$+ \int_{-L_o}^{+L_o} \phi_1^*(x)\left\{\frac{-\hbar^2}{2m_s}\left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial z^2}\right]\right\}\phi_2(x)\ dx$$

$$+ \int_{+L_o}^{+(L_o+a)} \phi_1^*(x)\left\{\frac{-\hbar^2}{2m_a}\left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial z^2}\right] - V_o\right\}\phi_2(x)\ dx$$

$$+ \int_{+(L_o+a)}^{+\infty} \phi_1^*(x)\left\{\frac{-\hbar^2}{2m_s}\left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial z^2}\right]\right\}\phi_2(x)\ dx$$

$$\Rightarrow \beta_{12} = E_2\int_{-\infty}^{-(L_\circ+a)} \phi_1^*(x)\phi_2(x)dx$$

$$+ \int_{-(L_\circ+a)}^{-L_\circ} \phi_1^*(x)\left\{\frac{-\hbar^2}{2m_a}\left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial z^2}\right] - V_\circ\right\}\phi_2(x)\ dx$$

$$+ E_2\int_{-L_\circ}^{+\infty} \phi_1^*(x)\phi_2(x)dx$$

Now,

$$\frac{m_s}{m_a}\int_{-(L_\circ+a)}^{-L_\circ} \phi_1^*(x)\left\{\frac{-\hbar^2}{2m_a}\ \frac{m_a}{m_s}\ \left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial z^2}\right] - V_\circ\right\}\phi_2(x)\ dx$$

$$= \frac{m_s}{m_a}E_2\int_{-(L_\circ+a)}^{-L_\circ} \phi_1^*(x)\phi_2(x)dx - V_\circ\int_{-(L_\circ+w)}^{-L_\circ} \phi_1^*(x)\phi_2(x)dx$$

and adding and subtracting $E_2\int_{-(L_\circ+a)}^{-L_\circ} \phi_1^*(x)\phi_1(x)dx$ gives:

$$\Rightarrow \beta_{12} = E_2\int_{-\infty}^{+\infty} \phi_1^*(x)\phi_2(x)dx + \left\{\left[\frac{m_s}{m_a} - 1\right]E_2 - V_\circ\right\}\int_{-(L_\circ+a)}^{-L_\circ} \phi_1^*(x)\phi_2(x)dx$$

$$= E_2\alpha_{12} + \left\{\left[\frac{m_s}{m_a} - 1\right]E_2 - V_\circ\right\}\int_{-(L_\circ+a)}^{-L_\circ} \phi_1^*(x)\phi_2(x)dx$$

Now we will make β a dimensionless quantity and equal to calculable quantities:

$$\frac{\beta_{12}}{\left[\hbar^2/\left[2m_a(a/2)^2\right]\right]} = \frac{2m_aE_2(a/2)^2}{\hbar^2}\alpha_{12} + \left[\left[\frac{m_s}{m_a} - 1\right]\frac{2m_aE_2(a/2)^2}{\hbar^2} - \frac{2m_aV_o(a/2)^2}{\hbar^2}\right]\int_{-(L_o+a)}^{-L_o}\phi_1^*(x)\phi_2(x)dx$$

$$= \gamma_2'^2\alpha_{12} + \left[(\epsilon-1)\gamma_2'^2 - \gamma_o^2\right]\int_{-(L_o+a)}^{-L_o}A\cos(kx)\bullet Be^{k'x}\,dx$$

$$= \gamma_2'^2\alpha_{12} + \left[(\epsilon-1)\gamma_2'^2 - \gamma_o^2\right]ABe^{-k'(L_o+a/2)}\left[\frac{e^{-k'L_o}}{k^2+k'^2}\left[k'\cos(ka/2)\bullet[1-e^{-k'a}] + k\sin(ka/2)\bullet[1+e^{-k'a}]\right]\right]$$

and recalling $\sigma = L_o/(a/2)$, $\frac{\beta_{12}}{\left[\hbar^2/\left[2m_a(a/2)^2\right]\right]}$

$$= \gamma_2'^2 + \left[(\epsilon-1)\gamma_2'^2 - \gamma_o^2\right](a/2)ABe^{-k'(\sigma+1)}\left[\frac{e^{-\sigma k'a/2}}{(ka/2)^2 + (k'a/2)^2}\bullet\left[(k'a/2)\cos(ka/2)\bullet(1-e^{-2k'a/2}) + (ka/2)\sin(ka/2)\bullet(1+e^{-2k'a/2})\right]\right]$$

$= \frac{\beta_{21}}{\left[\hbar^2/\left[2m_a(a/2)^2\right]\right]}$ via symmetry considerations (and noting that in the case of the double symmetric well, $\gamma_1'^2 = \gamma_2'^2$).