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THE
TRANSPORT PROPERTIES
OF
SEMICONDUCTOR SUPERLATTICES
AND
MULTIPLE QUANTUM WELL
STRUCTURES

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ABSTRACT

Electron transport perpendicular to the growth direction of two advanced semiconductor devices is studied, the superlattice and the multiple quantum well structure (MQW). Transport in these devices is dominated by the presence of very large electric fields which exist because these structures are inherently very thin.

The structures are formed using a growth technique such as Molecular Beam Epitaxy (MBE) where monolayers of one type of semiconductor material are literally grown on to another type of semiconductor. By ensuring that these two semiconductors have band gaps which are either of a different size or are not aligned, a series of quantum wells separated by barriers can be formed.

The MQW structure is treated as a fairly poor conductor with the electrons having a large probability of being inelastically scattered. Because of this strong scattering a formalism is developed that is flexible enough to include various scattering mechanisms with various scattering lengths. Conversely, the superlattice is treated as a fairly good conductor with a complete absence of inelastic scattering. This enables the electrons to be treated as perfectly coherent across the whole structure.

Optical absorption is also studied in a biased superlattice. This not only allows the energy states of the superlattice to be probed with great sensitivity, but the possibility also exists of using this system as an infrared detector.

Finally the effect of applying a weak magnetic field perpendicular to the electric field is also investigated as a means of reducing the amount of negative differential resistance that usually exists in the voltage-current characteristics of MQW structures.

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And finally I would like to save the biggest thanks of all for my wife Kate, THANKS.

A handwritten signature in cursive script that reads "James Leo." followed by a horizontal flourish line.

James Leo
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August 1988

"You see what I have done? I have transformed the problem from an intractably difficult and possibly quite insoluble conundrum into a mere linguistic puzzle. Albeit an intractably difficult and possibly insoluble one."

Dirk Gently P.I.

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1 INTRODUCTION

In any quantum mechanical system, the energy spectrum is characterised by the form of the potential energy. For instance, it was F Bloch who showed that a periodically varying potential produced well defined bands of energy levels comprised of plane waves separated by gaps in which it is forbidden for an energy state to exist. Furthermore, PW Anderson (1958) showed that a random or disordered potential structure would lead to a more interesting and rich spectrum, comprised of localised states characterised by a point spectrum and separated from extended states by a mobility edge.

However, a new hierarchy of system can be envisaged, in which the band edge is in some way artificially varied spatially. This will then, in turn, produce a new energy spectrum and hopefully one which can be fairly simply inferred from the previous one. This is exactly what has been achieved in Semiconductor Physics.

There are two ways in which the band edge of a semiconductor material can be made to vary spatially. The material can be doped with donors and acceptors which result in the formation of depletion regions resulting in internal electric fields. Alternatively, two materials that have energy bands and gaps that are positioned slightly differently, can be interfaced. This results in an abrupt discontinuity in the band edge across the interface forming a potential wall. However, the technological problems of forming a precise and definite interface between two semiconductor materials have been considerable and have led to the development of

sophisticated (and expensive) growth techniques. One of the most successful is Computer-controlled Molecular Beam Epitaxy (MBE) in which a directed beam of molecules and atoms created by effusion ovens are allowed to deposit on a substrate creating thin films of the required material. In order to achieve high quality epitaxy, it is vital that the system be enclosed in an ultrahigh vacuum ($\sim 10^{-10}$ Torr).

The work in this thesis will be concerned with a particular type of semiconductor structure. It is formed by growing several molecular (or mono) layers of a compound semiconductor using MBE, or one of its sister techniques, followed by several monolayers of another slightly different compound semiconductor. The idea then is to use two materials which have different band gaps. This can be achieved by varying the alloy composition in a semiconductor compound. Two materials which are frequently used in this respect, are AlGaAs and GaAs as AlGaAs has a wider band gap (WBG) than GaAs. By repeating the aforementioned growth process, a periodic system is constructed from alternating layers of narrow band gap (NBG) and WBG material. The WBG material will then confine allowed energy regions of the NBG material between potential walls to form wells. As the dimensions of these wells are in the quantum regime, quantised energy levels will form in each of the wells. The number of barriers or wells can then be preselected by growing the required number of sections of NBG and WBG material, Fig. 1.1. However, with MBE as with any other high technology the obtained results and the anticipated results are not always commensurate. These types of structure have been termed multiple quantum well (MQW) structures. Of course, the potential shown in Fig. 1.1 is only a crude oversimplification of the actual potential energy function that would be found in these structures. For a more realistic description see the papers by Bastard (1981 and 1983), Cade (1985), Altarelli (1983) and Marsh and Inkson (1986).

The novelty of these unique systems, which has caused

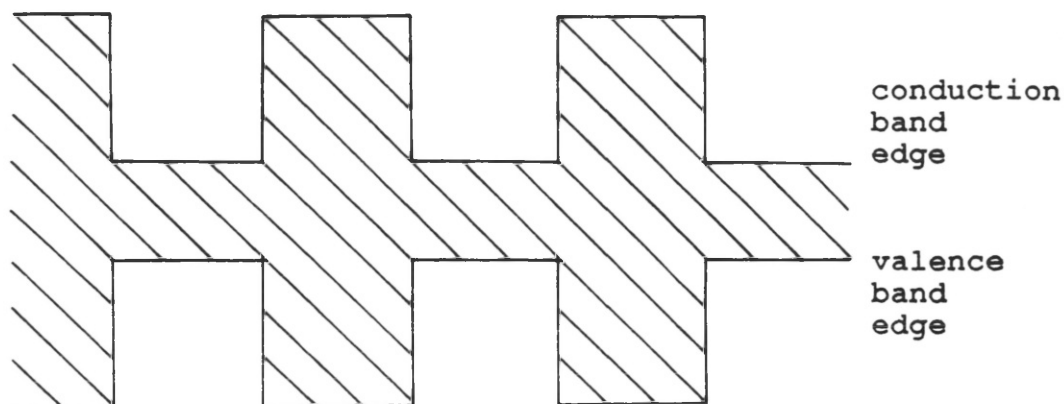


Fig. 1.1 Profile of the energy gap variation that results in the formation of a MQW structure. The shaded region represents the band gap.

so much research and attention to be focused on them, comes from several aspects of their quantum architecture. The first of these is that the widths of the barriers and wells, formed from the different materials, depend on the number of monolayers that are used. This means that because of the near monolayer accuracy that is becoming achievable with MBE, the barrier and well widths can be predetermined. This now gives rise to the possibility of tailoring the energy spectrum within certain limits. For instance, the widening of a well results in the lowering of the quantised energy states or even the formation of a new level. This effects the amount of mixing between neighbouring well states which in turn effects the amount of energy level splitting. Of course, the widths of the barriers also effect the amount of mixing. In fact because the barriers can be made sufficiently thick, the coupling between the wells or even between the wells and the electrodes of the device, can be reduced to a such an extent that the quantised well levels remain well defined and do not become totally smeared out. An alternative way

of viewing this is as a transport problem. By making the barriers relatively thick, the time taken for an electron that has just tunnelled into the well to tunnel out again can be made much larger than the time it takes the electron to cross from one side of the well to the other. Therefore, assuming that the scattering time is greater than either of the two aforementioned times, the electron will become completely aware of the confining effects of the well. Its wavefunction can then build up if the energy of the electron coincides with one of the quantised energy levels.

Although these systems have large scale structure in one dimension (the growth direction), they still maintain the properties of the host semiconductors in the other two dimensions, albeit within the confinements of a two dimensional system. This in itself leads to interesting properties. For example, the energy of the electrons has two components. Firstly there is the quantised energy due to the confining nature of the wells. Secondly there is the free-electron-like energy characterised by a perpendicular two dimension wavevector $k_{\perp}$. In fact the two dimensional electron gas (2DEG) as it is referred to, has been the focus of much scientific activity.

By increasing the number of wells and barriers in the system, a lattice structure can be built up. More importantly, this lattice can have a unit cell considerably larger than the unit cell of either of the two host semiconductors. Structures of this type have therefore been termed superlattices and their possible construction was first postulated by Esaki and Tsu in 1970. Making the barriers slightly narrower lifts the degeneracy that existed between the quantised energy levels in the thicker barrier devices mentioned above. This then results in the formation of bands, but because the barriers are still relatively thick and the wells are wide, these bands are very narrow so and have been termed minibands. Another way of viewing this is by considering the consequence of a large repeat length. It results in a very small Brillouin

zone. Therefore, the dispersion curves, which for a larger Brillouin zone extended beyond the new boundary, are folded back into the new zone resulting in the formation of more bands and gaps which are now narrower. For a more detailed description of the band structure of a superlattice, the reader is referred to the paper by Elci (1986) and references therein.

It has been postulated (Inoshita et al 1986 and Watanabe 1986) that in the future, the use of advanced microfabrication techniques could lead to the construction of a three dimensional analog of the superlattice, the so called super-superlattice constructed from arrays of superatoms. Although there has been some theoretical work on this system, the current state of technology precludes any experimental investigations, at least for the time being.

One property of MQW and superlattice structures that can have very dramatic and important effects is that they are very thin along the growth direction. Samples typically range in thickness from about $0.1\mu\text{m}$ to $5\mu\text{m}$. This means that even relatively small voltages applied perpendicular to the layers can produce very considerable electric fields. In most linear response theories of transport, the structural effect of the electric field on a system is neglected and only the effect it has on the charge carriers is included. For instance, the Drude theory of electrical conductivity in a metal gives the current j in terms of the field E as

$$j = \sigma E ; \quad \sigma = \frac{n e^2 \tau}{m^*} \quad (1.1)$$

where n is the conduction electron density, m^* is the effective mass and τ is the electron relaxation time. This theory may consider the flow of electrons through the system as a result of an applied electric field, but it does not consider any changes the electric field might induce in the electronic structure of the system. In the

theory of electrical transport in non-crystalline systems, the Kubo-Greenwood formula (Kubo 1956 Greenwood 1958) gives the conductivity for an electron moving in a disordered system, but again it neglects any effect the applied electric field might have on the electronic structure of the system. These and other theories are perfectly valid when the electric field is small, which is the case for many systems. However, the presence of the electric field on scales many times larger than that normally encountered warrants the use of new and modified techniques which must implicitly include the complete effect an electric field has on these ultrathin semiconductor devices.

This thesis contains a study of the transport characteristics of two classes of MQW/superlattice structure under the influence of large electric fields and in some cases magnetic fields as well. One type of structure is the Limited Coherence MQW (LCMQW). In this system the wavefunction of the electron is not coherent over the entire length of the system (i.e. the coherence length $L_c < L$ where L is the length of the system). This is because the phase of the electron gets randomised by it being involved in an inelastic collision as it travels across the sample. This category also includes structures which are very short, i.e. consisting of only two wells separated by a single barrier. In these types of structures, even if coherence is maintained over nearly the whole system, some type of scattering may be required so that the electron can release the energy it gained from the field and relax into an energy level. This type of scattering then may not play an important part in the transport characteristics.

The bulk of the experimental work has been concerned with devices that fall into this category. The Double Barrier Resonant Structure (DBRS) is one of the most studied (i.e. Goldman et al 1987, Reed and Lee 1987, Chang et al 1974, Capasso et al 1986a and Zou et al 1988). It is effectively characterised by its non-linear voltage-current (V-I) curves. These curves contain one or two regions of

negative differential resistance (NDR) due to the relative movement of the energy levels in the well and the Fermi level in the input-electrode region. When these match up, resonance occurs and the electrons can tunnel into the exit-electrode with almost no resistance causing a peak to occur in the current. However, changing the field results in the movement of the well levels causing a decrease in the current. The improvement of the peak to valley ratio in the NDR region has been of great concern to many workers as the possibility of using these devices as a logic gate has emerged. Therefore, at resonance the device can be said to be 'on' as a large current is flowing. However, at maximum mismatch, the current can be very small and then the device is 'off'.

Chapters 2 and 3 will contain the work on structures in this category. Chapter 2 will develop a transport formalism while Chapter 3 will use and extend the formalism to other more general situations.

The second type of structure is the Unlimited Coherence MQW (UCMQW). For the work contained in this thesis, this will refer to superlattices with well defined minibands so enabling research to be conducted from a viewpoint of how the electric field effects these minibands. However, this category could also contain any MQW structure of mesoscopic dimensions. There has not been anything like as much work conducted in the field of superlattices as has been on the DBRS. One of the prime reasons lies with the growth process. Producing high quality superlattices consisting of fifty or so periods is extremely difficult. Consequently, the production of shorter, simpler devices has been favoured. The original work on superlattices was undertaken by Esaki and Chang in 1974. Interesting and unexpected oscillations were discovered in the V-I curves and these will be discussed later. This work has recently been continued by Choi et al (1987a) and Vuong et al (1988) who also discovered similar effects to those found by the original workers. It should be noted here that although the superlattice has many

unique and interesting aspects, it is still a periodic lattice. Consequently, work that has involved studies of how periodic or even disordered lattices are effected by an electric field can still, within certain restrictions, be related to work carried out in this thesis. Furthermore, relevant work will be referred to and compared with the results obtained here.

Chapters 4, 5, 7 and 8 will form a study of both perfect and disordered superlattices under the influence of large electric fields. Chapter 6 will look at direct optical transitions in superlattices in the presence of electric fields while Chapter 9 will complete the thesis with a study of a magnetic field applied perpendicular to the electric field in a MQW structure.

Finally, in all the work carried out in this thesis, the effective mass approximation will be used. Any differences in the effective masses in the barrier and well regions will be neglected. Consequently, the differences between electron and hole (light or heavy) conduction will come from a change in the effective mass.

2 TRANSPORT IN COHERENCE LIMITED MQW STRUCTURES

2.1 Introduction

Previous studies of transport in MQW structures have tended to tackle the problem from a coherent tunnelling approach by assuming the system is of mesoscopic dimensions. That is, the electron is treated as an incoming plane wave characterised by two wavevectors, k_x and $k_{\perp}$. The electric field is in the x direction, perpendicular to the monolayers and so $k_{\perp}$ describes the wave in the two dimensional electron gas (2DEG). To obtain the current that is flowing in the device, the amplitude of the electron's wavefunction is calculated at the exit electrode given that no energy or momentum has been exchanged with the rest of the system (for example see Ricco and Azbel 1984). The condition of complete coherence can then be relaxed at the end points which act as sinks for the energy and momentum acquired from the field.

In this chapter, complete coherence of the wavefunction will not be required as a prior condition. In fact the contrary will be true and phase randomisation of the carrier's wavefunction as a result of some scattering event will be deemed to be extremely likely. The possibility now exists to divide transport across the structure into paths of various coherence lengths. This then enables the whole structure to be viewed as a series of resistors where each resistor corresponds to a configuration of barriers and wells, the length of the configuration representing the likelihood of being scattered. Any calculation requiring the total current

across the system would then need to include all the possible conduction paths in parallel. In the extreme case where the device consists of only a single well, it is the dimensions of the device and not scattering which restricts any long-range coherence. In fact, because of the device's length restriction in this case, only one conduction path will exist anyway.

The approach that the electron is most likely to relax some or all of its energy after a single step (i.e. crossing one barrier) is adopted. Longer range tunnelling paths can be subsequently included as higher order processes at a later stage if necessary. Therefore, transport across MQW systems is viewed as a highly sequential process. There has been some confusion in the literature caused by the use of the phrase 'sequential tunnelling' when referring to a very different transport process. In the papers by Price (1987), Weil and Vinter (1987) and Luryi (1985) sequential tunnelling is a term that refers to the way they study coherent tunnelling. The electrons are not involved in any scattering and move across the structure while preserving the phase of their wavefunctions. However, these authors view the electron as tunnelling from one well to the next. Although, when the electron reaches a well, it does not relax its energy, it merely exists in it for a time period before tunnelling on to the next. This process is, therefore, not the same as the one being studied in this chapter where there is a real exchange of the electron's energy with the system.

The above approach is clearly very powerful in that it permits the systematic inclusion of the totality of all scattering processes which normally would constitute an enormous complication. Experimentally it leads one to a very powerful point of view by which observed non-linear processes can be analysed systematically step by step by identifying sequential non-linearities from those due to longer range coherence. In this way the quality of a sample could be assessed by the weight of its long-range tunnelling paths.

2.2 The Double Well Model

Consider the simple double well potential structure given in Fig. 2.1 with a metallic contact to the left and right of the sample, so arranged that their resistances are Ohmic and much less than the resistance due to the barrier. The quantity ε_F denotes the Fermi level in the structure. The single well eigenstates for a well of thickness 'a' can be written (unnormalised)

$$\Phi_n = \begin{cases} e^{\alpha_o x} & x < 0 \\ \alpha_o^{-1} \sin[k(x-a/2) + n\pi/2] & 0 < x < a \\ (-1)^{n+1} e^{-\alpha_o (x-a)} & x > a \end{cases} \quad (2.1)$$

where ka tends to $n\pi$ as the well becomes infinitely deep, n is an integer and

$$\alpha_o^2 = \frac{2m^*}{\hbar^2} (V_o - E) \quad (2.2)$$

with V_o denoting the well depth, E the energy of the electron and $\hbar$ is Planck's constant. The box eigenvalues can be approximated by

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2m^* a^2} \quad (2.3)$$

The influence of neighbouring wells can be taken into consideration by introducing the tight-binding matrix elements

$$t_{n,m}(1,2) = \int_{-\infty}^{\infty} \Phi_{n,1}^*(x) V(x) \Phi_{m,2}(x - X_{12}) dx \quad (2.4)$$

where X_{12} is the distance between the well centres, 1 and 2 denote the well labels and $V(x)$ is the quantum well

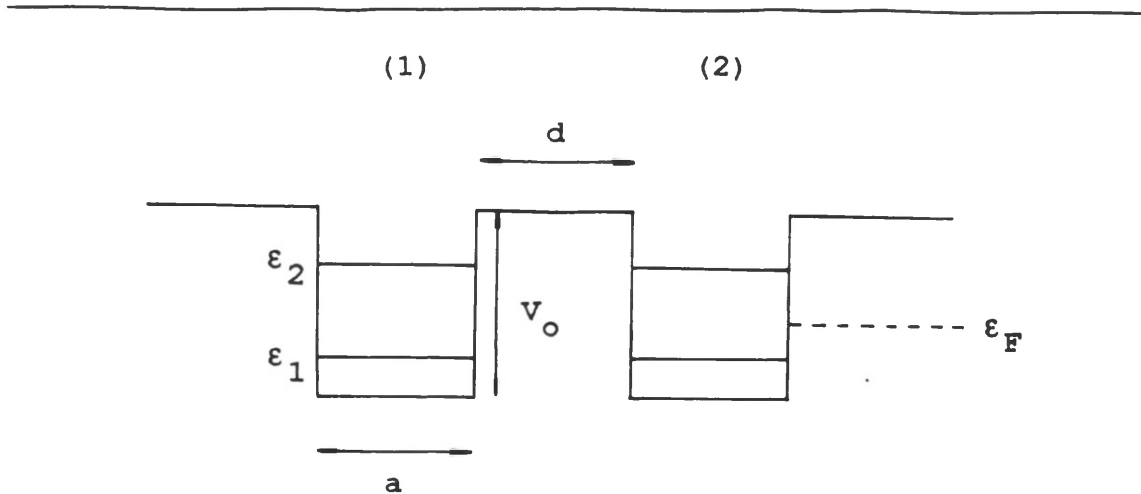


Fig. 2.1 The double well model. The Fermi energy ϵ_F shows the level of occupation of the states in the 2DEG.

potential as a function of position. To a good approximation

$$t_{n,m}(1,2) = V_0 e^{-K_m |X_{12}|} \quad (2.5)$$

where K_m is the smaller of the two inverse lengths given by Eq. (2.2). $t_{n,m}$ therefore leads to an admixture of all the eigenstates in the respective wells.

The presence of an electric field F leads to the situation illustrated in Fig. 2.2 where the band edges defining the barriers and wells are sloped with a gradient of eF (e is the electronic charge). Even from the tight-binding point of view, the situation is no longer so simple as it was because the solution of the well states in the presence of an electric field cannot be derived analytically. Good variational solutions have however been obtained by Bastard (1981 and 1983) and in principle these solutions could be used to evaluate the energies and the respective matrix elements. Instead, an approximation will be used that treats the electric field as a simple energy shift of eFd (d is the barrier width) between the

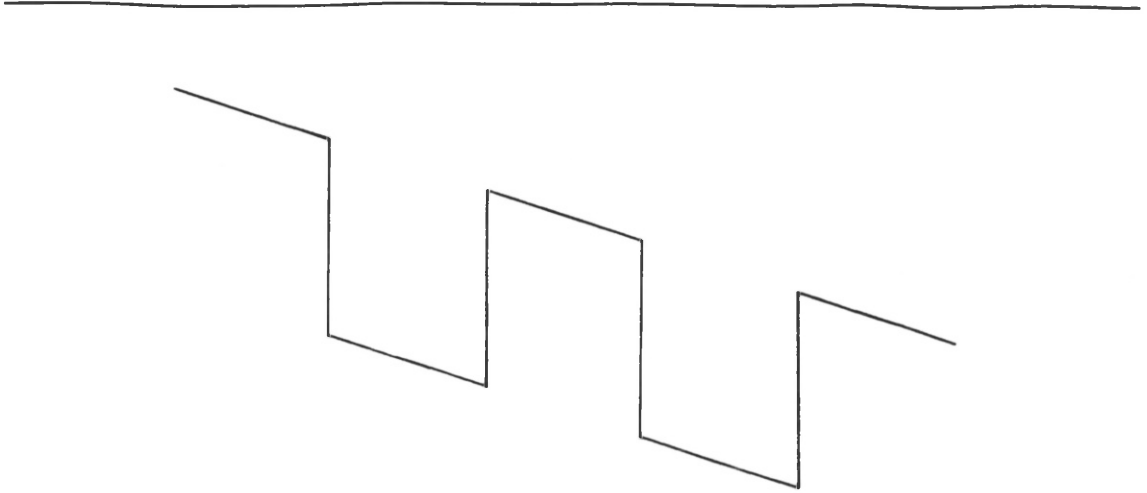


Fig. 2.2 The effect an applied electric field has on the double-well model shown in Fig. 2.1.

wells and neglects the field dependent changes in the matrix elements (Fig. 2.3). The double well wavefunction can now be written using the tight-binding approximation in terms of the unperturbed single well wavefunctions as

$$\Psi_n = \left[1 + \sum_m |\Gamma_{m,n}|^2 \right]^{-\frac{1}{2}} \left[\Phi_n(1) + \sum_m \Gamma_{m,n} \Phi_m(2) \right] \quad (2.6)$$

where the admixture coefficients $\Gamma_{m,n}$ are approximated by first-order perturbation theory. The resultant probability for the electron to be in level m in well[2] is

$$|\Gamma_{m,n}|^2 \left[1 + \sum_m |\Gamma_{m,n}|^2 \right]^{-1} \approx \frac{|t_{n,m}(1,2)|^2}{(\epsilon_m[2] - \epsilon_n[1])^2 + |t_{n,m}(1,2)|^2} \quad (2.7)$$

where $\epsilon_n[1]$ is the energy of level n in well[1] and $\epsilon_m[2]$ is the energy of level m in well[2] and can be written

$$\epsilon_m[2] = \epsilon_m^o[2] - eFd \quad (2.8)$$

where the 'o' denotes the zero-field case. The total

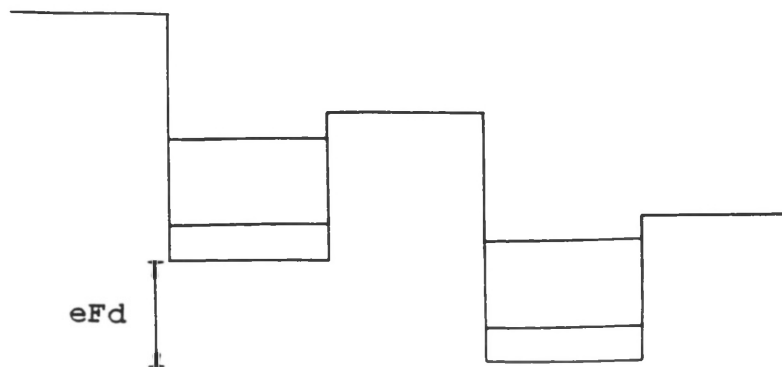


Fig. 2.3 The effect of the electric field is approximated by an energy shift of eFd between each well.

energy in this level is now

$$E_{m,\underline{k}}[2] = \varepsilon_m^0[2] - eFd + \varepsilon(\underline{k}) \quad (2.9)$$

where the perpendicular two dimensional free-electron energy has now been included.

The flexibility of the present formalism can be seen from Eq.(2.6). Although only a two well system is being considered, any size system could in principle be studied. This point will be returned to in the next chapter.

2.3 Well-Continuum Tunnelling

Above the bound states in the quantum wells is, to all intents and purposes, a continuous spectrum of unbound states. This spectrum may not be entirely continuous and small gaps could exist. However, these gaps will be ignored and for the present purpose these states will be taken as approximately plane wave like. In the presence of an electric field the plane waves states become Airy

functions of the type

$$A_c(Z) = \frac{1}{\pi} \int_0^{\infty} \cos \left[\frac{1}{3} s^3 + sZ \right] ds \quad (2.10)$$

where

$$Z = - \left[\frac{2m^* eF}{\hbar^2} \right]^{1/3} \left[x - \frac{E_c}{eF} - x_0 \right] \quad (2.11)$$

$x_0 = d$ and E_c are the continuous eigenvalues. The asymptotic forms of $A_c(Z)$ are

$$A_c(Z) \sim \frac{1}{\pi} \frac{1}{(Z)^{1/4}} e^{-(2/3)Z^{3/2}} \quad Z > 0 \quad (2.12)$$

$$A_c(Z) \sim \frac{1}{\pi} \frac{1}{(-Z)^{1/4}} \sin[(2/3)(-Z)^{3/2} + \pi/4] \quad Z < 0 \quad (2.13)$$

Given the rapid decay of the Airy wavefunction in the barrier, it is useful to assign to $A_c(Z)$ a localisation length, $\alpha_c^{-1}(F) = [\hbar^2 / (2m^* eF)]^{1/3}$ so that $A_c(Z)$ is negligible when $Z > 1$, i.e. $x\alpha_c > 1$.

In addition to the interwell coupling depicted in Eq.(2.4), there is also a coupling between well[1] and the continuum given by

$$T_{n,c}[1 \rightarrow c] = \int_{-\infty}^{\infty} \Phi_n^*(1, x) \{eFx\} A_c(x) dx \quad (2.14)$$

This term will give rise to tunnelling processes between the bound states of the well and the continuum of states outside the well. Such processes will be of importance for large values of F . The transition rate for this process is given by Fermi's Golden Rule as

$$\tau^{-1}(1, \varepsilon_n; c) = \frac{2\pi}{\hbar} |T_{n,c}[1 \rightarrow c]|^2 \delta(E_g^c - eF_B d - eF_S a_x n_c) \quad (2.15)$$

where E_g^C is the energy gap to the continuum, a_x is the lattice constant in the x direction and n_c is an integer. The field across the device has been separated into two components, the field across the barrier F_B and the field in the remaining part of the device F_s . The field F_s and F_B differ only when there is either doping in the system or a build up of space charge. An estimate of Eq. (2.15) gives

$$\tau^{-1}(1, \epsilon_n; c) = \frac{2\pi}{\hbar} \frac{1}{eFa_x} |eF\alpha_o^{-1}|^2 e^{-(2\alpha_o d + 2\alpha_c a_x n_c)} \quad (2.16)$$

where $n_c = (E_g^C - eF_B d) / eF_s$, α_o characterises the overlap between the quantum well wavefunctions and α_c characterises the transition from well[1] to the continuum Airy functions. When $a_x n_c \gg \alpha_c^{-1}(F)$ then $\alpha_c \equiv \alpha_o$ and the decay is always determined by the decay of the well states in the barrier.

2.4 Incoherent Interwell Tunnelling

As incoherence due to scattering is a prerequisite for tunnelling, the mechanisms which are responsible must now be studied. However, before doing this the philosophy behind the incorporation of scattering into the formalism set out in this chapter will be discussed.

Experimental data demonstrating clear regions of NDR in the V-I curves are commonplace nowadays and it has been discovered that increases in temperature tend to suppress these non-linearities while low temperature measurements have shown these features at their sharpest. This NDR has for some time been attributed to the mismatching of energy levels in neighbouring wells when an electric field is applied. Therefore, complete phase coherence across the barrier is needed for the levels in well[1] and in well[2] to couple to each other so that they can tell how far they are apart in energy. This then effects the probability of the electron being in one of the wells given in Eq. (2.7).

However, for the electron to remain in well[2], it must relax the energy it gained from the field. This can be accomplished via either an elastic or an inelastic interaction. In the elastic case, the total energy of the electron remains unchanged. Instead the electron changes its perpendicular two dimensional momentum allowing it to tunnel to the required energy state on the dispersion curve of well[2]. For the inelastic case, however, the electron relaxes by exchanging energy with either a phonon or with other electrons. Therefore, an element of both coherence and scattering are important.

As temperature increases, the 'washing out' of the NDR may be caused by these scattering mechanisms becoming dominant in the tunnelling process. Motion from well[1] to well[2] is, therefore, viewed as a two step process. The total rate is given by the product of two terms. The first term is the probability of coherently tunnelling across the barrier. It is this which is responsible for the NDR structure in the V-I curves. The second term is an inverse scattering time which characterises the particular scattering process. This term will become increasingly important under certain conditions depending on the scattering mechanism, i.e. increasing temperature for electron-phonon scattering, high impurity density for impurity scattering etc.

The transition rate from level n in well[1] to level m in well[2] is now written

$$W(1, \varepsilon_n; 2, \varepsilon_m) = |\Gamma_{m,n}|^2 \left[1 + \sum_m |\Gamma_{m,n}|^2 \right]^{-1} \frac{1}{\tau_{\text{scat}}} \quad (2.17)$$

where $1/\tau_{\text{scat}}$ is the intrawell inelastic scattering rate. The scattering rates for three likely mechanisms will now be calculated.

i) **The electron-phonon interaction:** The electron-phonon interaction can be written as (Fröhlich 1954)

$$H_{ep} = \sum_{\underline{q}, \mu} \{ C_{\mu}(\underline{q}) e^{i\underline{q} \cdot \underline{r}} b_{\underline{q}, \mu} + C_{\mu}^*(\underline{q}) e^{-i\underline{q} \cdot \underline{r}} b_{\underline{q}, \mu}^* \} \quad (2.18)$$

where $C_{\mu}(\underline{q})$ denotes the acoustic or optic coupling constant, μ the phonon branch index and the b 's are the creation and annihilation operators for phonons.

The electron has now tunnelled into well[2] with energy $\varepsilon_n[1] + \varepsilon_{\underline{k}}$ (the index 1 has been dropped for convenience and any $\underline{k}$ will be assumed to the momentum in the two dimensional perpendicular plane). It must now relinquish some energy to a phonon of momentum $\underline{q}$ and energy $\hbar\omega$ to be able to relax into the energy state $\varepsilon_m[2] + \varepsilon_{\underline{k}'}$, (note that $\varepsilon_m[2] = \varepsilon_m^0[2] - eFd$ from Eq. (2.8)). From Fermi's Golden Rule, the rate is given by

$$\frac{1}{\tau_{ep}} = \frac{2\pi}{\hbar} \sum_{\underline{k}', \underline{q}, \mu} \left[|H_{\underline{k}, \underline{k}'}^{n, m}(\underline{q})|^2 \delta(\varepsilon_{\underline{k}} + \varepsilon_n - \varepsilon_{\underline{k}'} - \varepsilon_m + \hbar\omega_{\mu}(\underline{q})) \times [1 - f(k')] |C_{\mu}(\underline{q})|^2 [n(\underline{q}) + 1] \right] \quad (2.19)$$

where

$$H_{\underline{k}, \underline{k}'}^{n, m}(\underline{q}) = \langle m | e^{-i\underline{q} \cdot \underline{x}} | n \rangle \delta_{\underline{k}, \underline{k}' + \underline{q}} \quad (2.20)$$

$|n\rangle$ is the one dimensional well wavefunction given by Eq. (2.1) and $n(\underline{q})$ is the phonon occupation number. ε_n will be assumed to be equal to ε_m where ε_m is the ground state quantum well energy. This is generally accepted as a possible transport mechanism (e.g see Capasso 1986a).

The acoustic phonon coupling constant is given by

$$C(\underline{q}) = iE_1 \left[\frac{q\hbar}{2\rho s} \right]^{1/2} \quad (2.21)$$

where ρ, E_1 and s are the density, deformation potential and

sound velocity respectively and for optic phonons the coupling is

$$C(\underline{q}) = \frac{iC}{\sqrt{\Omega}} \frac{1}{\underline{q}} \quad (2.22)$$

where

$$C^2 = 2\pi\hbar\omega e^2 \left[\frac{1}{\epsilon_{\infty}} - \frac{1}{\epsilon_0} \right] \quad (2.23)$$

ϵ_{∞} and ϵ_0 are the optical and static dielectric constants respectively and Ω is the volume.

To evaluate the acoustic phonon scattering rate, the dispersion of ω is taken to be linear, i.e. $\omega = sq$. This facilitates the calculations enormously and is a good approximation especially at small q when compared with theoretically predicted dispersion relations (i.e. for a GaAs/AlAs superlattice see Barker et al (1978)). The phonon occupation $n(q)$ is taken to be a Fermi distribution of the form

$$n(q) = (e^{\hbar\omega/k_B T} + 1)^{-1} \quad (2.24)$$

where k_B is Boltzmann's constant and $(1-f(k')) \approx 1$, which assumes that there is no restriction on the states available. The acoustic phonon relaxation rate can now be written

$$\frac{1}{\tau_{ep}} = \frac{2\pi}{\hbar} \sum_{\underline{k}', \underline{q}} \left[|C(\underline{q})|^2 [n(q)+1] f(q_x) \right. \\ \left. \times \delta_{\underline{k}, \underline{k}'+\underline{q}} \delta(\epsilon_{\underline{k}'} - \epsilon_{\underline{k}} + \hbar s q - e F d) \right] \quad (2.25)$$

where

$$f(q_x) = |\langle n | e^{-i q_x x} | n \rangle|^2 \quad (2.26)$$

After summing over $\underline{k}'$

$$\frac{1}{\tau_{ep}} = \frac{2\pi}{\hbar} \frac{1}{(2\pi)^2} \int_0^\infty q_\perp dq_\perp \int_{-\pi/a_x}^{\pi/a_x} dq_x \int_0^{2\pi} d\theta |C(\underline{q})|^2 (n(\underline{q})+1) \times \delta \left[\frac{\hbar^2 q_\perp^2}{2m^*} - \frac{\hbar^2 k_\perp q_\perp}{m^*} \cos\theta + \hbar s q - eFd \right] f(q_x) \quad (2.27)$$

which reduces to the following form after performing the $q_\perp$ and θ integrals in the small $\underline{k}$ limit

$$\frac{1}{\tau_{ep}} = \frac{1}{2\hbar} \left[\frac{E_1^2 \hbar}{2\rho s} \right] \int_{-\pi/a_x}^{\pi/a_x} f(q_x) dq_x \left[\left[\frac{2m^* eFd}{\hbar^2} \right]^{1/2} + \frac{k_B^T L}{\hbar s} \right] \quad (2.28)$$

As all the q_x dependence has now disappeared except for $f(q_x)$, the final integral can be evaluated quite simply. The single well states given in (2.1) are now substituted for $|n\rangle$ in Eq. (2.26) to give

$$\int_{-\pi/a_x}^{\pi/a_x} f(q_x) dq_x \approx \frac{2\pi}{a} + \frac{L^2 \pi}{3a^2} \quad (2.29)$$

where L is the well width. This gives the final form for the acoustic phonon scattering as

$$\frac{1}{\tau_{ep}} = \frac{1}{2\hbar} \left[\frac{2\pi}{a_x} + \frac{L^2 \pi}{3a_x^2} \right] \left[\frac{E_1^2 \hbar}{2\rho s} \right] \left[\left[\frac{2m^* eFd}{\hbar^2} \right]^{1/2} + \frac{k_B^T L}{\hbar s} \right] \quad (2.30)$$

This is an increasing function of field, but only quite weakly. The interesting point to note is that as the temperature increases, the field dependence tends to

disappear, i.e. when

$$\frac{k_B T_L}{s} \gg (2m^* eFd)^{1/2} \quad (2.31)$$

Another interesting point to make is that the temperature here is the effective lattice temperature T_L which is always non-zero when there is a current flowing. Depending on the electron-electron relaxation time in relation to the electron-phonon relaxation time, T_L can be greater than or less than T_e , the electron temperature.

For the evaluation of (2.19) in the optic phonon case, ω_μ is taken to be dispersionless. The scattering rate can be written in a similar form to (2.25) and after summing over k' the only difference from Eq.(2.27) that arises is that $\hbar s q - eFd$ is replaced by $\hbar \omega_\mu - eFd$. Now after performing the $q_\perp$ and θ integrals the scattering rate is given by

$$\frac{1}{\tau_{ep}} = \frac{2\pi}{\hbar} \frac{\pi C^2 m^*}{\Omega \hbar^2} [n(q) + 1] \times \int_{-\pi/a_x}^{\pi/a_x} f(q_x) \{q_x^4 + 4q_x^2(k^2 - \eta) + 4\eta^2\}^{-\frac{1}{2}} \theta(k^2 - \eta) dq_x \quad (2.32)$$

where $\eta = (m/\hbar^2) (\hbar \omega - eFd)$. The q_x integration is now very complicated and cannot be evaluated exactly. Therefore, suitable approximations are required if an analytical form is to be obtained for the optic phonon transition rate. The approximation that will be used here is to take two limiting forms for k , k very large and k very small. In this way the term under the square root in (2.32) can be sufficiently simplified to allow the integral to be evaluated.

The following two forms for the optic phonon transition rate were thus determined in the large k and small k limits

$$\frac{1}{\tau_{ep}} = \frac{2\pi^2 C^2 m^*}{\hbar^3 \Omega} [n(q)+1] \frac{1}{(k^2 - \eta)^{1/2}} \times \left[\ln \left[\frac{\pi (k^2 - \eta)^{\frac{1}{2}}}{\eta a_x} \left[\frac{\pi^2 (k^2 - \eta)}{\eta^2 a_x^2} + 1 \right]^{\frac{1}{2}} \right] + \frac{\pi^2}{2a_x^2} \right] \quad (2.33)$$

for $k^2 \gg \pi/a_x + \eta$

and

$$\frac{1}{\tau_{ep}} = \frac{2\pi^2 C^2 m^*}{\hbar^3 \Omega} [n(q)+1] \left[\frac{2\sqrt{2}}{\sqrt{\eta}} + 4 (k^2 - \eta)^{\frac{1}{2}} \right] \quad (2.34)$$

for $\pi/a_x + \eta \gg k^2$ and $k^2 > \eta$

For large k , increasing the field results in a decrease in the scattering rate, but when k is very small, the rate increases with the field. Therefore, there must be a crossover point at some specific value of k where the rate goes from an increasing to a decreasing function of field.

Electron-optic phonon scattering in a double well model has also been treated by Weil and Vinter (1986). These authors have numerically evaluated the effective interwell matrix elements while including the bonding-antibonding energy splitting. Their results for the scattering rates plotted against the voltage exhibit the features deduced in the approximate analytic formulae given above. An interesting point is that the computed scattering rates, $1/\tau_{ep}(\text{optic})$, lie in the range $(0.1-10) \times 10^{12} \text{ s}^{-1}$.

ii) The electron-electron interaction: When considering transport and relaxation processes, the density of carriers is an important consideration. If the density is high the carrier-carrier interaction can become the

dominant source of relaxation and therefore motion. It is, therefore, important to know how the electron-electron transition rates change as a function of the applied voltage.

Consider the interaction between an electron that has just tunnelled into well[2] with energy $\varepsilon_n + \varepsilon_{\underline{k}_0}$ and an electron that is in the two dimensional electron gas (2DEG) in well[2] with energy $\varepsilon_m + \varepsilon_{\underline{k}} - eFd$. The interaction leads to a transfer of momentum $\underline{q}$ so that the 2DEG becomes 'heated up' by electrons tunnelling in from well[1]. The interaction can be expressed by the Feynman graph in Fig. 2.4. The scattering rate can be written (again assuming $\varepsilon_n = \varepsilon_m$)

$$\frac{1}{\tau_{ee}} = \sum_{\underline{k}} \sum_{\underline{k}_0} \sum_{\underline{k}'} \frac{2\pi}{\hbar} |M(\underline{k}, \underline{k}_0 \rightarrow \underline{k}', \underline{k}_0)|^2 \{1-f(\underline{k}_0')\} \{1-f(\underline{k}')\} f(\underline{k}) \times \delta(\varepsilon_{\underline{k}_0'} + \varepsilon_{\underline{k}'} - \varepsilon_{\underline{k}_0} - \varepsilon_{\underline{k}} - eFd) \quad (2.35)$$

where

$$M(\underline{k}, \underline{k}_0 \rightarrow \underline{k}', \underline{k}_0) = \langle \underline{k}', \underline{k}_0' | V_{ee}(\underline{q}) | \underline{k}, \underline{k}_0 \rangle \quad (2.36)$$

The two dimensional screened electron-electron potential is given by (Ando et al 1982)

$$V_{ee}(\underline{q}) = \frac{2\pi e^2}{\varepsilon_s} \frac{1}{|\underline{q}| + |q_s(\underline{q})|} \quad (2.37)$$

where ε_s is the dielectric constant and $q_s(\underline{q})$ is the screening length given by

$$q_s(\underline{q}) = \bar{q}_s \left[1 - \left[1 - \frac{2k_F^2}{q^2} \right]^{\frac{1}{2}} \right] \quad (2.38)$$

and

$$\bar{q}_s = 2m^* e^2 / \varepsilon_s \hbar^2 \quad (2.39)$$

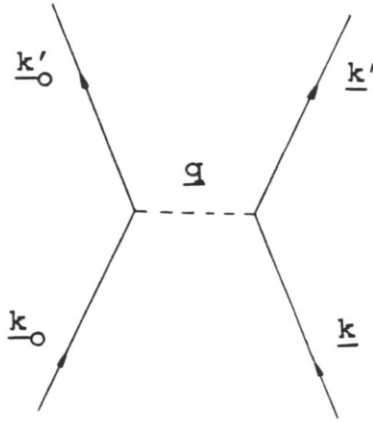


Fig. 2.4 A Feynman graph displaying the interaction between two electrons, one which has just tunnelled into well[2] from well[1].

The q dependence of the screening length reflects the fact that screening in two dimensions is very different to the three dimensional case. For simplicity, it will not be explicitly taken into account until the end of the calculation. In contrast to three dimensions, the screening of a charge Ze in a two dimensional quantum well is given by (Ando et al 1982 and references therein)

$$V_{ee}(r) \sim \frac{\sin(2k_F r)}{(2k_F r)^2} \frac{Ze\bar{q}_s}{\epsilon_s} \frac{4k_F^2}{(q_s + 2k_F)^2} \quad (2.40)$$

The weak $1/r^2$ decay is a result of the q -dependent screening length. By treating the two dimensional electron wavefunction as a plane wave, the scattering rate (2.35) can now be written

$$\frac{1}{\tau_{ee}} = \frac{2\pi}{\hbar} \sum_{\underline{k}} \sum_{\underline{k}_0} \sum_{\underline{k}'} \left[\{1-f(\underline{k}_0')\} \{1-f(\underline{k}')\} f(\underline{k}) |V_{ee}(\underline{k}_0 - \underline{k}_0')|^2 \right. \\ \left. \times \delta(\underline{k}_0' + \underline{k}' - \underline{k}_0 - \underline{k}) \delta(\epsilon_{\underline{k}_0'} + \epsilon_{\underline{k}'} - \epsilon_{\underline{k}_0} - \epsilon_{\underline{k}} - eFd) \right] \quad (2.41)$$

In the limit that the field energy $eFd \gg \varepsilon_{\underline{k}_0}$, to a good approximation the rate can be written

$$\frac{1}{\tau_{ee}} = \frac{2\pi}{\hbar} \frac{1}{4\pi^2} \left[\frac{2\pi e^2}{\varepsilon_s} \right]^2 \frac{4m^*}{\hbar^2 (q_s + q_F)^2} n_c \quad (2.42)$$

where n_c is the carrier density in the well, $eFd = \hbar^2 q_F^2 / 2m^*$ and $q_s(q_c)$ is the screening length evaluated at the critical value q_c . This rate can further be approximated to give

$$\frac{1}{\tau_{ee}} = \frac{2\pi}{\hbar} \frac{1}{4\pi^2} \left[\frac{2\pi e^2}{\varepsilon_s} \right]^2 \frac{2}{E} n_c \quad (2.42)$$

where E is the total energy of the electron when it arrives in well [2]. Note the proportionality to electron density and the inverse proportionality to total energy E which for the present case if $eFd \gg \varepsilon_{\underline{k}_0}$ is $\sim eFd$. Therefore, Eq. (2.42) suggests that an increase in F leads to a 'slowing down' of the electron-electron relaxation rate at high fields.

iii) Impurity scattering: As was mentioned at the start of this section, the electron crossing the barrier does not have to relax its energy inelastically, it can scatter elastically and exchange the energy it gained from the electric field with its perpendicular two dimensional kinetic energy. Therefore the energy conservation relation

$$\varepsilon_{\underline{k}} + \varepsilon_n^0[1] = \varepsilon_{\underline{k}'} + \varepsilon_m^0[2] - eFd \quad (2.43)$$

is satisfied by a change in momentum given by

$$eFd = \frac{\hbar^2}{2m^*} (\underline{k}'^2 - \underline{k}^2) \quad (2.44)$$

Scattering processes capable of supplying such a momentum change are charged impurities (dopants), well-width fluctuations or disorder in the barrier layers (i.e. AlGaAs). However, when dopants are present in sufficiently high concentrations ($N_d \sim 10^{17}$ or more) these

become the dominant scattering mechanism. If they are present in the wells, then the process can be viewed as a two step process. Therefore the scattering rate is

$$\frac{1}{\tau_{\text{imp}}} = \frac{2\pi}{\hbar} \sum_{\underline{k}'} |V_i(\underline{k}-\underline{k}')|^2 \delta(\epsilon_n[1] + \epsilon_{\underline{k}} - \epsilon_n[2] - \epsilon_{\underline{k}'}) \quad (2.45)$$

where $V_i(\underline{q})$ is the Fourier Transform of the elastic scattering potential $V_i(r)$ (see Sawaki and Akasaki 1985) and n has been taken to be equal to m , i.e. the electron is tunnelling from ground state to ground state.

All the inelastic two step processes can now be summarised in a total direct transition rate $w_{1,2}^{n,m}(\underline{k})$ between the two quantum wells as

$$w_{1,2}^{n,m}(\underline{k}) = \left[\frac{1}{\tau_{\text{ee}}}(\underline{k}) + \frac{1}{\tau_{\text{imp}}}(\underline{k}) + \frac{1}{\tau_{\text{ep}}}(\underline{k}) \right] \times \frac{|t_{n,m}(1,2)|^2}{(\epsilon_m^0[2] - \epsilon_n^0[1] - eFd)^2 + |t_{n,m}(1,2)|^2 + \Delta^2(\underline{k})} \quad (2.46)$$

where $\Delta^2(\underline{k})$ represents the lifetime broadening due to $\underline{k}$ scattering in the two dimensional plane of the quantum well.

What happens when transport across the barrier is viewed as a single step, direct process? Consider the impurity scattering process treated above. If the dopants are in the barrier, then it is very likely the electron will be scattered as it crosses. This is now viewed as a single step process by writing down the scattering rate between a state $\epsilon_{n,\underline{k}}$ in well[1] and a state $\epsilon_{m,\underline{k}'}$ in well[2] as

$$\frac{1}{\tau}(\underline{k}) = \frac{2\pi}{\hbar} \int d\underline{k}' |\langle \epsilon_m[2], \underline{k}' | V_{\text{imp}} | \underline{k}, \epsilon_n[1] \rangle|^2 \times \delta(\epsilon_m[2] + \epsilon_{\underline{k}'} - \epsilon_n[1] - \epsilon_{\underline{k}}) \quad (2.47)$$

where

$$V_{\text{imp}} = \sum_n \frac{-e^2}{4\pi |\underline{r} - \underline{R}_n| \epsilon_s} e^{-q_s |\underline{R}_n|} \quad (2.48)$$

is the screened impurity potential, q_s is the inverse screening length and ϵ_s is the dielectric constant. In contrast to the case of the electron-electron interaction within a well, the three dimensional screening form is used. This is because now interwell scattering is being considered. An approximate evaluation of (2.47) gives

$$\frac{1}{\tau}(\underline{k}) = \frac{\pi^2}{\hbar} \frac{2m^*}{\hbar^2} \frac{e^2}{4\pi\epsilon_s} e^{-2\alpha_0 d} \times \left[\left[k^2 + \frac{2m^* e F d}{\hbar^2} \right]^{\frac{1}{2}} - k + q_s \right]^{-2} N_{\text{imp}} \quad (2.49)$$

where N_{imp} is the impurity density α_0 is given by (2.2) for $E = \epsilon_n[1]$.

The major difference between the direct process and the two step process is that Eq.(2.46) has a rather strong voltage dependence because of the separate tunnelling factor. This is not so for the direct impurity induced transition. In fact (2.49) tends to suppress the electric field dependence of the resistance altogether whereas the scattering given by (2.45) will give a substantial NDR effect. This has interesting consequences as to the role of disorder. Disorder, which is predominantly responsible for the processes in (2.46) will not therefore, destroy the NDR in the V-I characteristics. However, direct transitions of the type given by (2.49) will if predominant, destroy most of the structure in the V-I curves.

2.5 The Interwell Current

The total current flowing across the barrier can now be found using the transition rates that were calculated previously. However, the back current that may exist against the field and the occupancy of the states in the wells must also be taken into account. Therefore the current is given by

$$I_{12} = de \sum_{\underline{k}, \underline{k}'} \sum_{n, m} \left[f(E_{n, \underline{k}}[1]) \{1 - f(E_{m, \underline{k}'}[2])\} W_{1, 2}^{n, m}(\underline{k}, \underline{k}') \right. \\ \left. - f(E_{m, \underline{k}'}[1]) \{1 - f(E_{n, \underline{k}}[1])\} W_{2, 1}^{m, n}(\underline{k}', \underline{k}) \right] \quad (2.50)$$

where $W_{1, 2}^{n, m}(\underline{k}, \underline{k}')$ denotes the sum over all possible interwell transition rates by which a carrier starts from well[1] in energy state ϵ_n with perpendicular momentum $\underline{k}$ and ends up in well[2] in the energy state ϵ_m with momentum $\underline{k}'$. The Fermi functions involve the effective temperature T_{eff} .

To a good approximation, (2.50) can be replaced by the following simpler expression

$$I_{12} = de \sum_{\underline{k}} \sum_{n, m} \left[f(E_{n, \underline{k}}[1]) W_{1, 2}^{n, m}(\underline{k}) \right] \\ \times \{1 - e^{-eFd/k_B T_{\text{eff}}}\} \quad (2.51)$$

where the sum over $\underline{k}'$ has been carried out and detailed balance has been invoked, i.e.

$$W_{1, 2}^{n, m}(\underline{k}, \underline{k}') = W_{2, 1}^{m, n}(\underline{k}', \underline{k}) e^{-|E_m - E_n|/k_B T_e} \quad (2.52)$$

The rate $W_{1, 2}^{n, m}(\underline{k}, \underline{k}')$ may involve the potential drop across the barrier as in Eq.(2.46) and is the main source of non-linear (non-Ohmic) behaviour in the present model.

2.6 Conclusion

The focus of this chapter has been the building of the foundations of a transport formalism for MQW structures where coherence of the electron's wavefunction is of no great consequence beyond the nearest-neighbour quantum well. By studying the relatively simple (but also at times very complicated to treat) double well structure, many of the salient features of transport have been covered in a, hopefully, perspicuous fashion while highlighting the underlying physics.

To include all the essential features of electron transport across the single barrier, the current was treated as a superposition of two processes. A resonant tunnelling contribution which can decrease or increase due to the energy levels separating or moving closer under the influence of the field. This results in the regions of NDR that are so characteristic of these systems. The second contribution comes from inelastic scattering of the carrier after it has tunneled into well[2]. This type of formalism not only allows the reproduction of the attractive NDR features, but also includes the scattering induced suppression of the NDR.

3 SEQUENTIAL AND DEEP LEVEL ASSISTED TUNNELLING

3.1 Introduction

This chapter extends the work started in the last chapter. Instead of treating transport across a single barrier only, transport that may be coherent over several well/barrier periods or even over the whole structure will now be investigated. A formalism, that is a simple extension of the one covered in chapter 2, will be constructed. This formalism will then be used, not to study longer structures, but to study a slightly different very important problem of the effect of deep levels, that may be located in the barrier layers, on the tunnel current across a barrier.

3.2 Variable range coherent tunnelling

In Eq.(2.6) the wavefunction for the double well structure was written down using the tight-binding approximation. However if a sum over wells is included, it then becomes the wavefunction for a many well system. Therefore the wavefunction for a system of v wells is

$$\Psi_n = \left[1 + \sum_v \sum_m |\Gamma_{m,v}|^2 \right]^{-\frac{1}{2}} \left[\Phi_n(1) + \sum_v \sum_m \Gamma_{m,v} \Phi_m(v) \right] \quad (3.1)$$

where $\Gamma_{m,v}$ is the admixture between level m in well $[v]$ and all the other levels in all the other wells. The corresponding probability, therefore, for the electron to

be in level m in well $[v]$ is

$$\frac{|\Gamma_{m,v}|^2}{1 + \sum_v \sum_m |\Gamma_{m,v}|^2} \quad (3.2)$$

There are two ways the coefficients Γ can be calculated. One way is to construct the Schrödinger equation for the system of wells in the following matrix form

$$\begin{bmatrix} \epsilon_1 & t_{12} & t_{13} & t_{14} & \cdot & \cdot \\ t_{21} & \epsilon_2 & t_{23} & t_{24} & \cdot & \cdot \\ t_{31} & t_{32} & \epsilon_3 & t_{34} & \cdot & \cdot \\ t_{41} & t_{42} & t_{43} & \epsilon_4 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix} \begin{bmatrix} 1 \\ a \\ b \\ c \\ \cdot \\ \cdot \end{bmatrix} = E \begin{bmatrix} 1 \\ a \\ b \\ c \\ \cdot \\ \cdot \end{bmatrix} \quad (3.3)$$

where the diagonal elements are the unperturbed eigenenergies in each well and the t 's are the matrix elements between the eigenstates. If, for instance, each well has two energy levels then the above matrix represents a two well model. This eigenvalue problem can now be solved using standard matrix techniques. For a three well problem, each with only one energy level the coefficients are given by

$$a = \frac{t_{12}}{(E - \epsilon_2) - \Sigma} ; \quad b = \frac{t_{12}}{(E - \epsilon_2 - \Sigma)} \frac{t_{23}}{(E - \epsilon_3)} \quad (3.4)$$

$$\text{where the self-energy } \Sigma = \frac{|t_{23}|^2}{E - \epsilon_3}$$

It has been assumed that the matrix was symmetric so $t_{12} = t_{21}$. As the systems get longer or the number of energy levels in each well gets larger, the solution of (3.3) gets rapidly harder. In fact solving matrices bigger than 4×4 may be straightforward but is extremely tedious and time consuming. Therefore for larger systems the Renormalised Perturbation Expansion (Economou 1983) is used to obtain

the coefficients. This is basically just a set rules for the determination of the coefficients. To simplify calculations further, only nearest neighbour interactions are included. This is a good approximation because of the relative thickness of the barriers.

The influence of the electric field is included in the same way as the last chapter. It is viewed as an energy shift of eFd between each well. This has come to be known as the 'ladder approximation' because the energy states of the wells form a ladder. It has been used by other workers (Cota et al 1985, Schwartz and Ting 1987) who have also found it to be a good approximation and it will be used again later in this thesis.

So now with this approximation the solution of (3.3) does not become any more complicated. All that needs to be changed is that the diagonal elements of the matrix have to be shifted by integer multiples of eFd . Therefore

$$\begin{aligned}\epsilon_1 &\rightarrow \epsilon_1 \\ \epsilon_2 &\rightarrow \epsilon_2 - eFd \\ \epsilon_3 &\rightarrow \epsilon_3 - 2eFd \\ &\text{etc.}\end{aligned}$$

If L_c the coherence length is shorter than L , the length of the system, transport becomes sequential for the electrons due to phase randomisation caused by inelastic scattering. Eq.(3.1) no longer describes a wavefunction for the whole MQW structure but only includes wells within a length L_c . This scattering event is characterised by a time τ_{inel} and can be due to any of the processes described in the last chapter. Using the technique formulated in the last chapter, a scattering rate can be calculated. This is obtained from a product of the inelastic scattering time τ_{inel} and the probability of being at the position of scattering (see Eq.(2.17)). Another wavefunction can now be constructed from this position to the next scattering position a distance L_c away again using (3.1). From there another scattering time can be calculated and so on.

Therefore the structure has been divided up into 'phase-coherent sub-sections', each one characterised by a scattering rate.

From this series of rates, a single rate is required representing motion across the entire system. The total rate is given by the reciprocal of the time it takes the electrons to cross the entire system. This is then given by the sum of the times it takes the electrons to cross each phase-coherent sub-section. Therefore

$$\tau_{\text{tot}} = \sum_i \tau_i \quad (3.5)$$

where the τ_i 's include both the inelastic scattering time and the probability (as in Eq.(2.17)) as well as the occupancy of the initial and final states in the phase-coherent sub-section. The total rate is thus given by

$$W_{\text{tot}} = \frac{1}{\tau_{\text{tot}}} = \frac{1}{\sum_i \tau_i} \quad (3.6)$$

The total current can then be calculated using Eq.(2.50) and (2.51) by including the back current and the occupancy of the initial and final states.

3.3 Deep Level Assisted Tunnelling

Deep levels that may be located in the barrier layers of the MQW structure in sufficient numbers can have a dramatic effect on the tunnelling current. Experimental evidence of this has been reported by Capasso et al (1986b) in a fifty period AlInAs/GaInAs structure in which they observed a series of peaks in the low temperature photocurrent. They attributed this to tunnelling via the deep levels in the barrier layers of their structure. Many other workers may not have observed these very pronounced resonances in the current, but they may be seeing a

consequence of deep level tunnelling when they observe a 'washing out' of the NDR at high temperatures.

Consider a single deep level located in the barrier of the double well structure in Fig. 2.1. The inclusion of this extra state can be viewed as splitting the barrier into two parts to effectively form a third quantum well between well[1] and well[2]. However, it should be noted that the wavefunctions of this 'third quantum well' are localised in all three spatial dimensions unlike those of well[1] and well[2] which are only restricted in one dimension and are plane waves parallel to the layers of the quantum well structure. This deep level can be used as a path of conductance across the structure in the following two ways:-

i) The direct process: In this process the electron uses the deep level states as a stepping stone to cross from well[1] to well[2]. The tunnelling probability can then be calculated from Eq.(3.1) where states from well[1], well[2] and the deep level are included. The probability of tunnelling across the whole structure is then given by the coefficient of the final state. The total rate can then be calculated by including the appropriate inelastic scattering time.

ii) The indirect process: Now consider the effect if the inelastic scattering length is shorter than the width of the barrier. The process of going from well[1] to well[2] is now a sequential or indirect process. If there are deep levels in the barrier, carriers can relax the energy gained from the field at those sites before tunnelling across the rest of the barrier. Therefore, there are now two inelastic scattering events that have to be included when calculating the total transition rate. As coherence is now only maintained between the well states and the barrier impurity, two wavefunctions must be written down describing each phase-coherent sub-section as outlined in the last section. So for this process, two probabilities and two scattering times are needed.

To study both of the above processes, only the

tunnelling probability will be calculated. This is considered to be the important quantity because of its strong voltage dependence which leads to the NDR. The inelastic scattering time is merely treated as a multiplying factor. Also, for the indirect process where the electron relaxes its energy at the deep level, only the step of going from the initial well to the deep level will be considered. This is because the rate in (3.6) can be approximated by the reciprocal of the longest time. The time taken to tunnel to the deep level will usually be longer than the time it takes for the electron to tunnel out. This is because this level is higher than the initial level at most biases. Consequently, some kind of activation energy is required. Also there is not the large number of states available in the deep level as are available in the wells because of the two dimensional density of plane wave states.

Although it may seem that well[2] has been ignored, its presence within the total structure is still required. Consider for instance the deep level being higher up in energy than the initial state in well[1]. In this case a current would not necessarily flow between well[1] and the deep level. However, the presence of a level in well[2] that is lower in energy than the initial level in well[1] would then allow a current to flow.

To first try and reproduce the experimental results of Capasso et al where distinct resonances are observed in the tunnel current, only tunnelling from a single state in well[1] rather than from a Fermi distribution of states is considered. For all the calculations in this chapter the energies of the well states were set to 0.1eV, the barrier height to 0.6eV and $t=0.01\text{eV}$. Fig.3.1 shows the results for the tunnelling probability at a temperature of 77K via the direct process when there is one deep level, E_d , located near the top of the barrier. Note that the abscissa on this graph is the voltage drop across the whole structure shown in Fig.2.1. Two distinct peaks can be clearly observed. The one at low voltages is caused by the initial level in well[1] resonating with the final level in well[2] However because the barrier is fairly wide the peak is

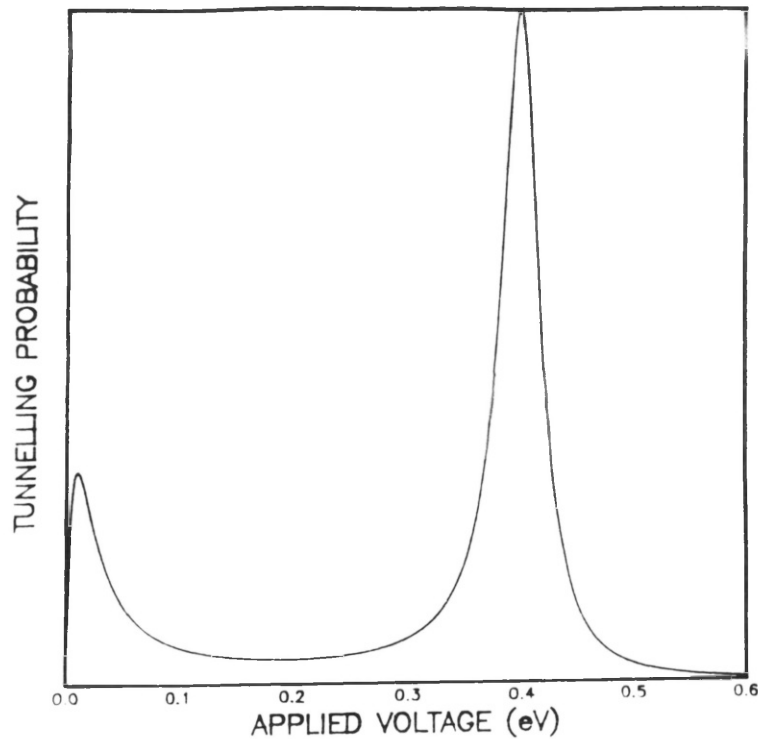


Fig. 3.1 The tunnelling probability for the direct process via a single deep level plotted against voltage at $T=77K$. ($E_B=0.3eV$)

consequently not very high. However, as the voltage across the structure is increased the initial and final levels go off resonance and eventually the deep level comes into resonance with the initial level. It is interesting to note that the initial linear rise in the tunnelling probability seen in Fig. 3.1 up to about $0.02eV$ is what would only be observed in a linear response type theory when Ohm's law is valid.

Fig. 3.2 shows the results for the indirect process with all the conditions equivalent to those in Fig. 3.1. But now because the electron relaxes its energy at the deep level before it reaches the final state in well[2], there is no initial peak in the tunnel current. Both Figs. 3.1 and 3.2 illustrate how deep levels located in the barrier could produce the sharp resonances obtained by Capasso et

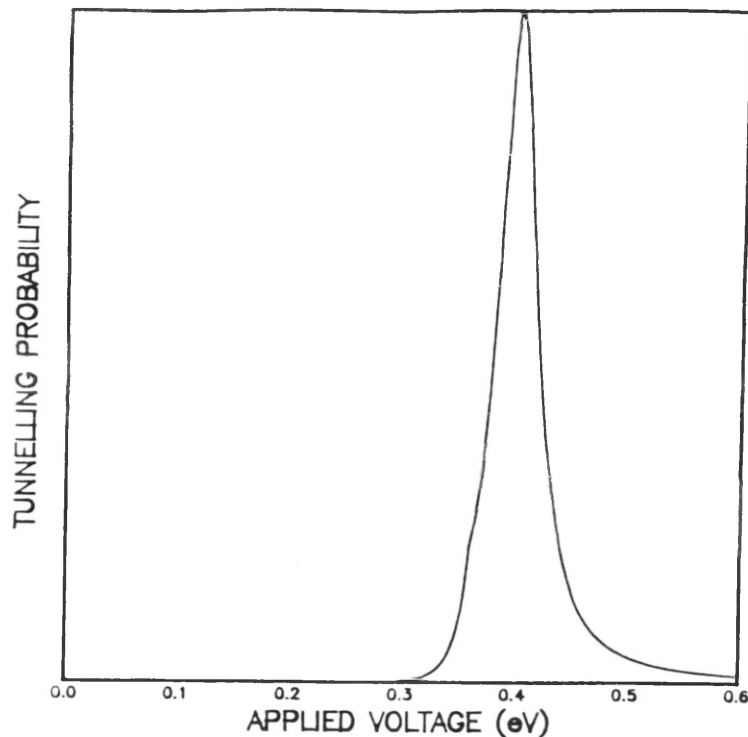


Fig. 3.2 The tunnelling probability for the indirect process via a single deep level plotted against voltage at $T=77\text{K}$. ($E_B=0.3\text{eV}$)

al.

Now consider how deep level assisted tunnelling can effect the temperature dependence of the NDR and even lead to its total disappearance by considering a Fermi distribution of states in the wells. At low temperatures the Fermi distribution of electrons is fairly constant up to the Fermi energy. However a rise in the temperature of the structure may result in the electrons having a larger spread of energies and therefore being able to access higher energies in the conduction band. These 'excited' electrons can now use the higher lying deep levels as conducting paths across the barrier and so enable a larger current to flow. Even when there is maximum misalignment between the energy levels in neighbouring wells, a significant tunnel current can still exist via these deep

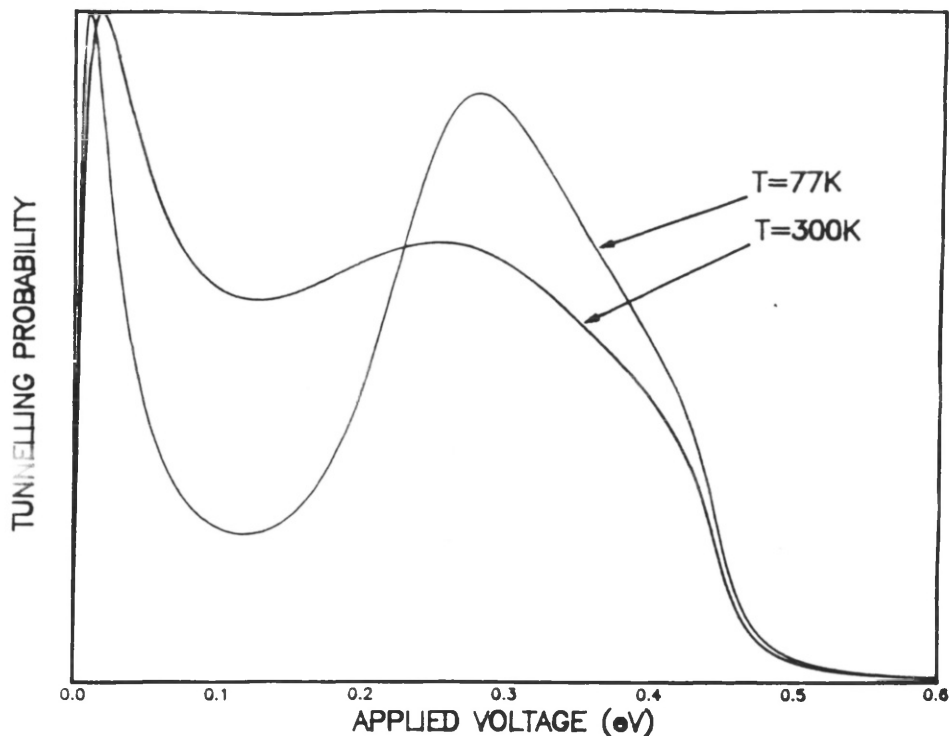


Fig. 3.3 The tunnelling probability for the direct process with a Fermi distribution of initial states plotted against voltage at $T=77\text{K}$ and $T=300\text{K}$. ($E_g=0.3\text{eV}$)

levels. Therefore the effect of the energy level misalignment is dramatically reduced which consequently results in a 'washing-out' or reduction of the NDR in the V-I characteristics.

Fig. 3.3 shows the results for direct tunnelling across the barrier using a single deep level located near the top of the barrier when there is a Fermi distribution of initial states ($\epsilon_F=0.4\text{eV}$). At 77K both peaks are clearly visible as they were in Fig. 3.1. However as the temperature is increased to 300K , both peaks are smeared out into one much broader peak. Fig. 3.4 shows the results for the indirect process under the same conditions as Fig. 3.3. The effect of temperature now seems to be less dramatic, however, there is a significant increase in the tunnelling probability at lower fields.

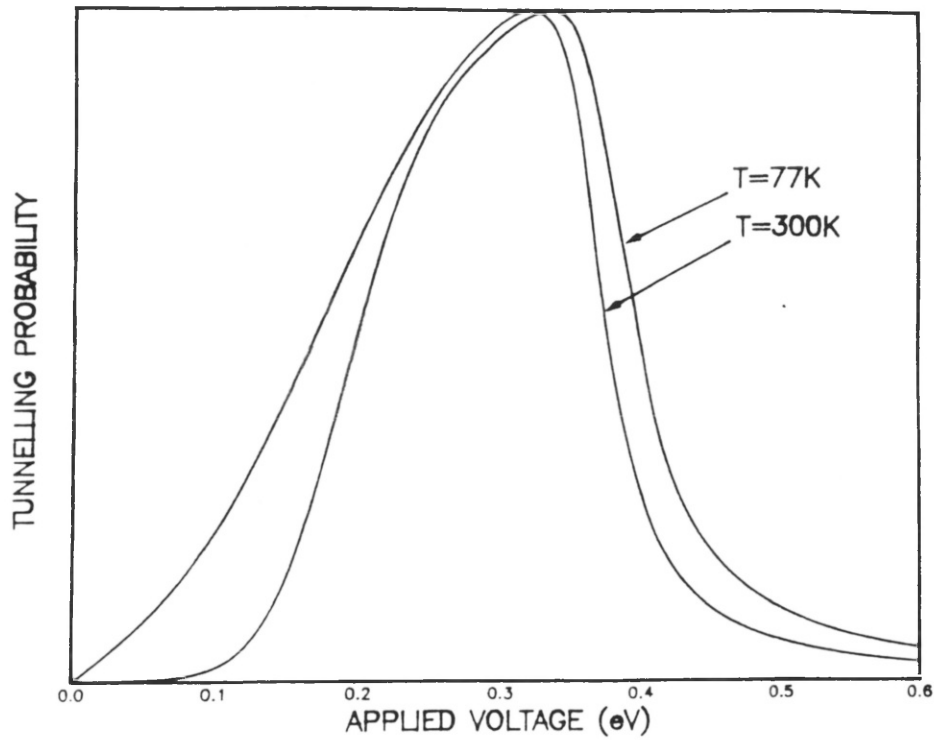


Fig. 3.4 The tunnelling probability for the indirect process with a Fermi distribution of initial states plotted against voltage at $T=77\text{K}$ and $T=300\text{K}$. ($E_g = 0.3\text{eV}$)

The way deep levels were represented above can be for one of two cases. A single impurity located in the barrier or for a whole line of impurities located along the barrier, i.e. a δ -doping effect. If the single impurity case is considered, electrons that are some distance away from the impurity level might not be expected to use it to cross the barrier. Therefore, the maximum distance the electrons can be from this level to make it more favourable to travel to it and then cross the barrier rather than simply crossing the barrier is needed. This will then give an estimate of the lower limit on the density of impurities in the barrier, n_{imp} , needed to significantly effect the system.

Let t_1 be the time taken to cross the barrier without the impurity state and t_2 be the time taken to cross with

the impurity. Therefore for the impurities to be of importance to transport the following inequality must hold

$$t_1 > t_2 + \frac{L^2}{D} \quad (3.7)$$

where L is the distance the electron is from the impurity and D is the diffusion constant and is given by

$$D = \frac{\mu k_B T}{e} \quad (3.8)$$

where μ is the mobility, T the temperature, k_B Boltzmann's constant and e the electronic charge. If for GaAs a value of $\mu=50,000 \text{ cm}^2/\text{Vs}$ is taken, then for the impurity states in the barrier to appreciably effect transport $n_{\text{imp}} > 10^{10} \text{ cm}^{-3}$ at 77K. It would seem therefore that a high density of impurities is not required in the barrier to significantly effect the transport of electrons.

Future work in this area could include the study of deep levels with internal structure. A negative or positive Hubbard U could then be assigned to the impurity level depending on whether the presence of an electron in that state lowered its energy or increased its energy. An example of a negative U state could be a DX centre in AlGaAs (for example see Kobayashi et al 1985). Occupancy of the impurity levels could then become important if the time it takes for an electron to leave the level exceeds the time taken for another electron to arrive. Then only an electron with an opposite spin to that which the electron already on the level has could use the level to cross the barrier. Implantation of either a single deep level or arrays of deep levels in the barrier layers (doping or δ -doping) would result, if the dopants were of a suitable type, in the following effective Hamiltonian

$$\begin{aligned}
H = & \sum_{n,\mu,\sigma} \varepsilon_{n,\sigma}^{\mu}(\underline{k}) c_{n,\sigma}^{\dagger}(\mu,\underline{k}) c_{n,\sigma}(\mu,\underline{k}) \\
& + \sum_{\sigma} \varepsilon_{d,\sigma} c_{d,\sigma}^{\dagger} c_{d,\sigma} + U n_{d\uparrow} n_{d\downarrow} \\
& + \sum_{n,\mu,\sigma} [V_{n,d}(\mu,\underline{k}) c_{n,\sigma}^{\dagger}(\mu,\underline{k}) c_{d,\sigma} + \text{c.c.}] \quad (3.9)
\end{aligned}$$

where $\varepsilon_{d,\sigma}$ represents the deep level energy (in analogy to the famous Anderson Hamiltonian for magnetic impurities), $\varepsilon_{n,\sigma}^{\mu}(\underline{k})$ is the energy of an electron in well μ with spin σ , U is the electron-electron repulsion which results in any doubly occupied states being shifted into an 'interesting' energy region for resonant tunnelling, and finally $V_{n,d}(\mu,\underline{k})$ represents the electron-deep level interaction. The simplicity of the above Hamiltonian is somewhat deceptive because in reality it represents a full scale many-body problem via the spin memory of the deep levels. Strong magnetic fields and microwaves may therefore modulate the tunnel current in suitably designed structures. One could then also start thinking about using 'magnetic layers' to produce spin polarised currents by spin-dependent tunnelling. A detailed discussion of this effect is, however, beyond the scope of this thesis.

3.4 Γ -X Tunnelling Transitions

For barrier materials with indirect energy gaps (X band in AlAs and compounds), tunnelling processes can take place mixing states of different symmetry (Γ -X transitions). These tunnel processes have been studied in detail experimentally by Mendez et al (1986) and Pritchard et al (unpublished) and theoretically by Ko and Inkson (1988) and Bonnefoi et al (1988). They can be of importance for thin barriers and in certain energy ranges. The Γ -X coupling in GaAs/AlAs systems has been estimated using optical techniques by Meynadier et al (1988). Usually a tunnelling transition involving Γ -X crossing requires a

momentum change which has to be compensated by a phonon or by an impurity interaction. This point has been discussed by Mendez. Transitions involving X-states can therefore be treated within the present formalism as 'transitions' involving a deep level of energy E_x (known for different alloy compositions) with coupling energy Γ_x (an equivalent quantity to the tight-binding coupling t_{12}).

In contrast to deep level assisted tunnelling, Γ -X crossing can in principle take place at any point in the well, i.e. the carrier does not have to move laterally until it finds a suitable crossing point, and so there is obviously no configurational averaging involved. If important, such effects should therefore show up as definite resonances in the I-V characteristics. In practice because the magnitude of the coupling $\Gamma_x \sim 3-40$ meV, such processes are often difficult to distinguish from lifetime broadening processes ($\Gamma \sim 0.1$ ps for an optic phonon energy relaxation process, giving a broadening of ~ 10 meV). However Γ -X tunnelling does seem to play a major role in the washing out of the NDR in pressure experiments.

3.5 Conclusion

This chapter has been concerned with the extension of the work in the last chapter to include systems, other than the simple double well structure, which have inelastic scattering lengths shorter than the length of the system. If however, $L_c > L$, then although this formalism is adequate another method, like the transfer matrix method, might be more appropriate. In fact this method will be used to study completely phase coherent superlattices in chapters 7 and 8.

The effects of deep levels in the barrier layers has also been studied. Deep levels constitute an important problem in tunnelling, not just from a point of view of an annoyance that needs to be eliminated, but they should also be viewed as a potential for obtaining new physics.

4 STARK-WANNIER STATES AND STARK LADDERS IN SUPERLATTICES

4.1 Introduction

In this, and the next four chapters, the emphasis will move away from short, poorly coupled MQW systems with large amounts of inelastic scattering. Instead, long coherent superlattices with well formed minibands will be studied.

As was mentioned earlier, superlattices in the growth direction are not much different from any other one dimensional periodic system. Therefore, the majority of this chapter will be concerned with reviewing the theory of periodic systems under the influence of large electric fields. Following this there will be a discussion on how this then relates to a superlattice in the presence of large electric fields.

4.2 Consequences of an Electric Field on a Periodic System

The effect of a substantial electric field applied across a periodic structure was first investigated by Zener (1934) who used the sloping band picture (Fig. 4.1) to study electrical breakdown in solids caused by electrons crossing from the valence band to the conduction band, an effect now termed Zener tunnelling. The concept of a Stark ladder was introduced some years later by Wannier (1954, 1960) to explain the energy spectrum of states within these sloping bands. It is derived by writing the Schrödinger equation for a periodic system in the presence of an

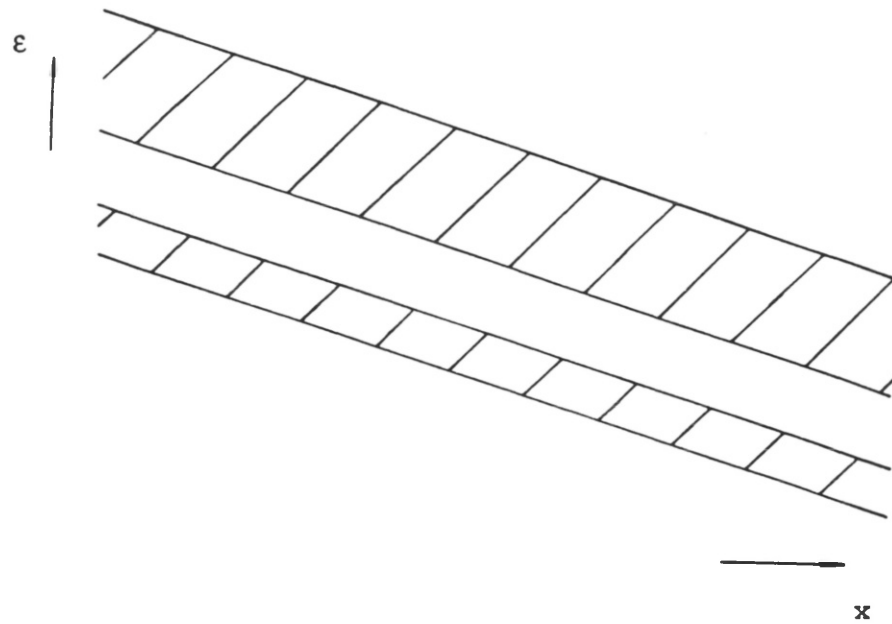


Fig. 4.1 Energy versus position diagram showing the effect an electric field has on the bands of a periodic system. The shaded areas represent the allowed energy regions.

applied electric field as

$$\left[\frac{p^2}{2m} + V(x) - eFx \right] \Psi(x) = E \Psi(x) \quad (4.1)$$

As $V(x+a)=V(x)$, a translation of Eq.(4.1) by a lattice constant 'a', gives

$$\left[\frac{p^2}{2m} + V(x) - eFx \right] \Psi(x+a) = (E+eFa) \Psi(x+a) \quad (4.2)$$

Therefore, for any state located at an energy E , there is an identical state located at a shifted energy $E+eFa$ with the same wavefunction except that its position is displaced by a lattice constant. In fact Eq.(4.1) can be translated by any number of lattice constants to eventually form the

familiar Stark ladder given by

$$E_m = eFam + E_0 \quad (4.3)$$

where m labels the Stark state and E_0 denotes the energy origin of the ladder.

Therefore, the basic requirement exists that every energy level must belong to a ladder and that the states of the ladder are spatially shifted relative to one another by integer multiples of the lattice constant. In fact, it will be shown later that there is a one to one relationship between each state in the ladder and each unit cell. It is not required, however, that every energy level must belong to the same ladder. Indeed this can not always be possible if the above requirements are to be satisfied. In a system with only one energy band, all the Stark levels will belong to the same ladder. The inclusion of an extra band will result in another Stark ladder being formed to incorporate the extra energy levels. In the context of the sloping band picture, each band can be viewed as being comprised of a Stark ladder of energy states.

To understand how these banded Stark ladders interact with each other, again consider the Schrödinger equation given in Eq.(4.1). The Stark-Wannier wavefunctions can be written as superpositions of Bloch states

$$\Psi(x) = \sum_{n',k'} C(n',k') |n',k'\rangle \quad (4.4)$$

Substituting (4.4) into (4.1) and multiplying through by the Bloch state $\langle n,k|$ gives

$$[\varepsilon(n,k) - E]C(n,k) = eF \sum_{n',k'} \langle n,k|x|n',k'\rangle C(n',k') \quad (4.5)$$

where $\varepsilon(n,k)$ is the Bloch energy. The matrix element can

now be written (Saitoh 1972)

$$\langle n, k | x | n', k' \rangle = i \delta_{n, n'} \delta_{k, k'} \frac{\partial}{\partial k} + \delta_{k, k'} X_{n, n'} \quad (4.6)$$

where

$$X_{n, n'} = iN \int_0^a e^{i(k' - k)x} u_{nk}^*(x) \frac{\partial}{\partial k'} u_{n'k'}(x) dx \quad (4.7)$$

$u_{nk}(x)$ is the periodic part of the Bloch function and the integral is only over a unit cell.

The effective Schrödinger equation now has the form

$$[\varepsilon(n, k) - E] C(n, k) = ieF \frac{\partial}{\partial k} C(n, k) + eF \sum_{n'} X_{n, n'} C(n', k) \quad (4.8)$$

The important term here is the matrix element $X_{n, n'}$ which couples the bands together. In the paper by Saitoh, this term was neglected to enable a study of a single band system to be made. Using the tight-binding approximation and ignoring the individual well wavefunctions, Saitoh derived the Stark-Wannier wavefunction to be

$$\Psi(x) = \frac{1}{\sqrt{a}} J_{x/a - m} \left[\frac{W/2}{eFa} \right] \quad (4.9)$$

where $J_n(x)$ is the Bessel function of the first kind and W is the band width. This now shows that an electron in the m 'th state of the single band Stark ladder is centred around $x=ma$, and localised within a length W/eF called the Stark length L_s . The more general form of the Stark-Wannier wavefunction which includes the well wavefunctions will be used later in this thesis. The zero point energy of the Stark ladder E_0 was also derived for the single band model and found to be

$$E_0 = \frac{a}{2\pi} \int_{-\pi/a}^{\pi/a} \varepsilon(k) dk \quad (4.10)$$

where $\varepsilon(k)$ is the dispersion relation for the unperturbed system.

In order to carry out a complete multiband analysis, it is important to include the interband term $X_{n,n'}$, when solving (4.8) to allow for Zener tunnelling between bands. This will then permit the delocalisation of electrons. However, there has been some controversy about whether this matrix element between the bands actually exists (Wannier 1950, 1955 and Kane 1959). Fukuyama et al (1973) have studied this problem briefly using a two band model and have concluded that two interpenetrating Stark ladders do exist and that they are coupled together. This is a very important point as an absence of any interband coupling could dramatically reduce the transport of electrons through the system.

Furthermore, Emin and Hart (1987) have attempted to solve the problem of a multiband system analytically. They divide the effect of an electric field on a one dimensional chain of N square well potentials in an electric field into two components. One component alters the shape of each potential well whilst the other shifts each one by an energy eFa relative to its neighbour (the ladder approximation). The first effect can then be included into the system's periodic potential to form a basis of electric field dependent Bloch states and the second effect can be represented by a Step function in the Hamiltonian. The matrix element given in Eq.(4.5) can be rewritten in the following way to represent the effect splitting the field into the two components has on the interband coupling.

$$\begin{aligned}
 \langle n, k | x | n', k' \rangle &= \int_0^{Na} e^{i(k'-k)x} u_{nk}^*(x) x u_{n',k'}(x) dx \\
 &= \sum_{m=0}^{N-1} e^{i(k'-k)ma} \int_0^a e^{i(k'-k)x} u_{nk}^*(x) x u_{n',k'}(x) dx \\
 &+ \sum_{m=0}^{N-1} m e^{i(k'-k)ma} \int_0^a e^{i(k'-k)x} u_{nk}^*(x) u_{n',k'}(x) dx \quad (4.11)
 \end{aligned}$$

As a **finite** system is being considered, the following equation

$$\sum_{m=0}^{N-1} e^{i(k'-k)ma} = N \delta_{k,k'} \quad (4.12)$$

is an exact relation for the k 's that satisfy

$$k = \frac{2\pi}{Na} n \quad \text{where } n \text{ is an integer} \quad (4.13)$$

The k 's therefore form a complete representation of the finite system. Where necessary, Eq.(4.12) should be treated as the definition of the Kronecker delta. The matrix element can now be written

$$\begin{aligned} \langle n, k | x | n', k' \rangle &= N \delta_{k,k'} \int_0^a u_{nk}^*(x) x u_{n',k}(x) dx \\ &\quad - i \frac{N}{a} \frac{\partial}{\partial k'} \left[\delta_{k,k'} \right] I(n, k; n', k') \end{aligned} \quad (4.14)$$

where

$$I(n, k; n', k') = \int_0^a e^{i(k'-k)x} u_{nk}^*(x) u_{n',k'}(x) dx \quad (4.15)$$

The first term in Eq.(4.14) contains the component of the field that alters the shapes of the wells while the second term results from the Step function potential which shifts each well relative to its neighbour. The second term can be written in the following way

$$i \frac{N}{a} \left[\delta_{k,k'} \frac{\partial}{\partial k'} I(n, k; n', k') - \frac{\partial}{\partial k'} \left[\delta_{k,k'} I(n, k; n', k') \right] \right] \quad (4.16)$$

Emin and Hart then show that after summing over k' and n' , the first term is zero and the second gives no interband coupling. They therefore conclude that it is the effect of the electric field on the shapes of the wells that gives

the interband coupling. However, their conclusion is wrong because of an error in their calculations. This will be investigated further in the next chapter.

Other work in the area of Stark ladders and Stark states has been carried out by Nagai and Kondo (1980) who numerically calculated the wavefunctions of a infinite Kronig-Penny model in an electric field; Bentosela et al (1982) who used a semi-infinite Kronig-Penny model in an electric field to study the Stark ladder energies (or resonances as they refer to them); Avron (1982) who looked at the lifetime (or width) of the Stark states; José et al (1985) who studied the energy levels of a random chain of delta-functions in an electric field; Bentosela (1985) who also studied a disordered chain of delta-function potentials and finally Pacheco and Claro (1988) who calculated the density of states of a finite periodic system in an electric field.

4.3 Stark-Wannier States and Stark Ladders in Superlattices

Much of the above work on electric field effects has been something of an academic exercise in theoretical physics. This is because in most ordinary systems the Stark ladders and Stark states probably, to all intents and purposes, do not exist, and even if they did, their observation would be near impossible. The reason for this is that it is very difficult to form a Stark state that is weakly coupled to any other states either in other bands or outside the sample. To prevent the state from being strongly coupled to the edges of the sample, the Stark length L_s must be much shorter than the length of the system. As $L_s = W/eFa$, either the band must be narrow or the field must be large. But for most practical systems the band width and the size of available fields result in very long Stark lengths.

Therefore, an ideal system for forming Stark ladders would have narrow bands, be able to sustain large electric

fields to enhance Stark localisation and also have a wide band gap to stop strong interband tunnelling which could broaden out the Stark states. A system which has these properties is the semiconductor superlattice. Consequently, transport in a superlattice has already been considered from the Stark ladder/state point of view (i.e. see Movaghar 1987).

In the paper by Esaki and Chang (1974), the band widths and gaps were calculated for varying well widths in an AlAs/GaAs superlattice. For a well width of around $45\text{\AA}$ the band width of the valence band was less than 0.01eV , the band gap was 0.2eV and the conduction band was 0.04eV . Compare this to something like Silicon which has a valence band width of 10eV . Therefore the Stark length will be orders of magnitude less in a superlattice. Also as superlattices are very thin ($\sim 1\text{ }\mu\text{m}$) the electric fields that can be obtained are very large for fairly standard voltages.

Also the fact that these structures are man-made means that the band widths and gaps can be optimised to some degree to increase the likelihood of observing the effects of the Stark ladders and states. Namely, to produce narrow bands needed to minimise the Stark length, the barrier widths can be widened, but to regulate the amount of band mixing, the well widths can be made narrower to form a larger band gap.

The above theory of Stark ladders in superlattices also assumes that the electric field is uniformly dropped across the whole system. This means that there are no high field domains which could result in all or the majority of the field being dropped across one part of the structure. This, however, is what has been observed in many superlattice structures (Esaki and Chang 1974, Kawamura et al 1986, Choi et al 1987a and Vuong et al 1988) where oscillations in the current are attributed to the movement of a high field domain through the sample. Therefore, to avoid this happening, one would require a structure similar to that used by Capasso et al (1986c). In their 35 period

superlattice they observe regions of negative differential resistance in the photocurrent which they conclude are not the result of high field domain formation. This is because their structure is of the type $n^+ - i - p^+$. Therefore, it has a natural built in bias but does not permit the flow of electrons. To obtain a current, a He-Ne laser is used to create electrons as minority carriers in the p^+ layer. The field across the superlattice can then be changed by applying a reverse bias.

5 THE DOUBLE MINIBAND SUPERLATTICE

5.1 Introduction

In the last chapter many of the principles in the theory of periodic systems in an electric field were reviewed. However, there has not been much work on multiband systems or more precisely multiband superlattices. This is reflected in the apparent confusion in the literature when claims are still made that the energy bands of a periodic system are not coupled under the influence of an electric field.

To understand the interaction between energy bands more fully a two band tight-binding Hamiltonian in the presence of a very large electric field is studied. This work could then relate to a two miniband superlattice or indeed any periodic system. A two band model is used as it contains all the essential physics of interband coupling without the problems associated with a complete multiband analysis. A two band model in an electric field has also been studied by McMurray and Falicov (1980) although they used a very different two band model (see Franz 1956). The use of more than two bands would just make the situation more complicated without introducing any new concepts. This work should then clarify some of the unresolved aspects of how bands couple in an electric field.

5.2 The Model

The energy spectrum and the wavefunctions of a

periodic two band system in the presence of an electric field can be explicitly calculated using a one dimensional nearest neighbour tight-binding model. Two states are defined on each site i , an s -state $|i,s\rangle$ and a p -state $|i,p\rangle$ both of which are tightly bound onto that site. The Hamiltonian representing a two band system can therefore be written as

$$\begin{aligned}
 H = & \sum_i \varepsilon_s |i,s\rangle\langle s,i| - V_s \left[|i-1,s\rangle\langle s,i| + |i,s\rangle\langle s,i+1| \right] \\
 & + \sum_i \varepsilon_p |i,p\rangle\langle p,i| - V_p \left[|i-1,p\rangle\langle p,i| + |i,p\rangle\langle p,i+1| \right] \\
 & + \sum_i V_{sp} \left[|i-1,s\rangle\langle p,i| + |i,s\rangle\langle p,i+1| \right] \\
 & - \sum_i V_{sp} \left[|i-1,p\rangle\langle s,i| + |i,p\rangle\langle s,i+1| \right] \quad (5.1)
 \end{aligned}$$

where ε_s and ε_p correspond to the on-site energies of the s and p orbitals, V_s and V_p correspond to the matrix element between s and p orbitals respectively and V_{sp} is the matrix element between an s orbital and its neighbouring p orbital. To form two bands where the second band is wider than the first and the gap between them is of the order of the band widths the following values were used; $\varepsilon_s=0$, $\varepsilon_p=14$, $V_s=1$, $V_p=3$ and $V_{sp}=2$. This results in the width of the lower band, which shall be referred to as the s -band, being 4 and the width of the upper band, the p -band, being 12. The resulting band gap was 6. To simulate the effect of the electric field, each on-site energy was perturbed by eFi where e is the electronic charge which was set to one, F the field strength and i the site label (the ladder approximation).

Although the two bands are referred to as s -bands and p -bands, these bands are never comprised of states that are purely s -like or p -like, but of a mixture. Of course, in the absence of an electric field, the s -band does contain

more s-like states than p-like states and similarly for the p-band.

5.3 Results

Fig. 5.1 is an energy level diagram obtained by diagonalising the Hamiltonian given in Eq.(5.1) at $F=1.265$. The two interpenetrating Stark ladders are clearly discernible and the spacing between the energy levels in each of the ladders is eFa . This is therefore in total agreement with the result obtained by Fukuyama et al (1973) who also showed that two interpenetrating Stark ladders exist in a two band system. It should be noted here that the energy levels given in Fig. 5.1 are only a selection which represent the energy spectrum in the bulk material. Energy levels that lie at the extremes of this energy spectrum are affected by the edges of the sample. This will consequently result in a modification of the energy spacing between the Stark levels.

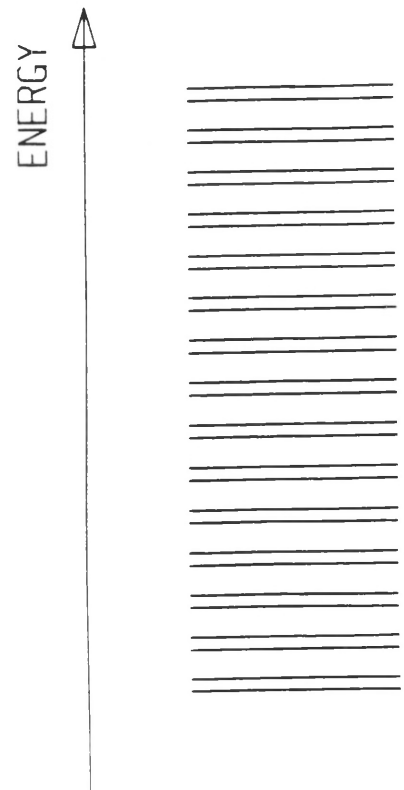


Fig. 5.1 The energy spectrum of the two band tight-binding model. The two interpenetrating Stark ladders are clearly visible.

To confirm the validity of viewing the Stark ladders as belonging to separate bands, the wavefunction of two neighbouring energy states were calculated, each one belonging to one of the ladders given in Fig. 5.1. It can

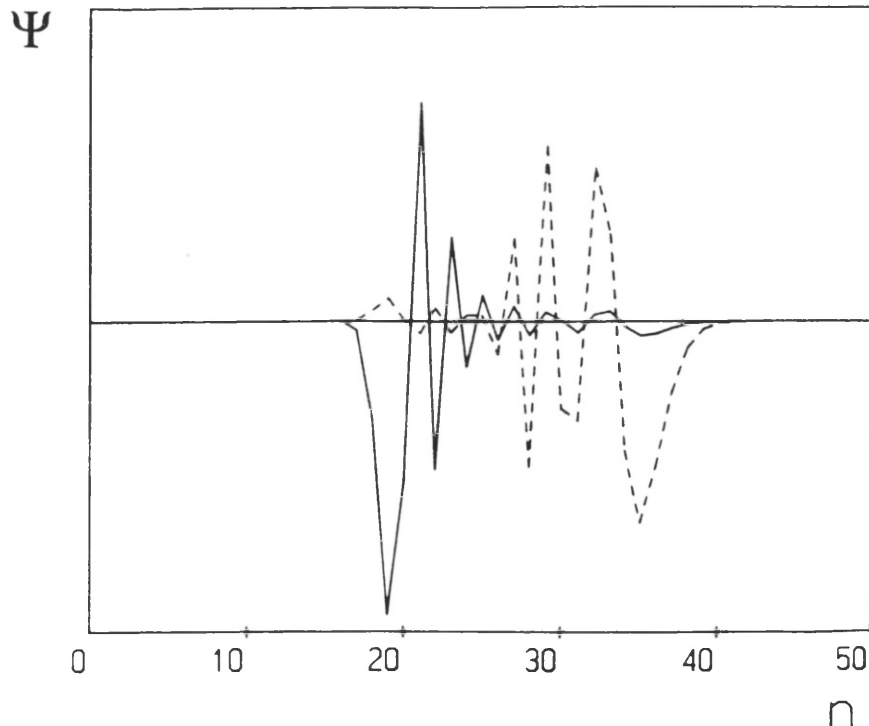


Fig. 5.2 The Stark-Wannier wavefunctions at $F=1.236$. Notice how their centres are spatially shifted relative to each other.

clearly be seen from Fig. 5.2 that each wavefunction has its maximum centred on different points. By referring back to Fig. 4.1, it can be seen that a state which belongs to one of the bands has its centre or its point of maximum amplitude shifted relative to a state that belongs to the other band. Therefore, from Fig. 5.2 it can be concluded that the wavefunctions, and therefore the Stark ladders, do belong to different bands.

Furthermore, consider the spatial extent of the wavefunction. In Fig. 5.2 each wavefunction covers about 20 sites. The Stark length at a field of 1.265 and with a band width of 22 (this includes both bands and the gap) is 17.4. It therefore seems that the wavefunctions straddle both bands. But it is also clear in Fig. 5.2 that the wavefunction represented by a dotted line has a longer

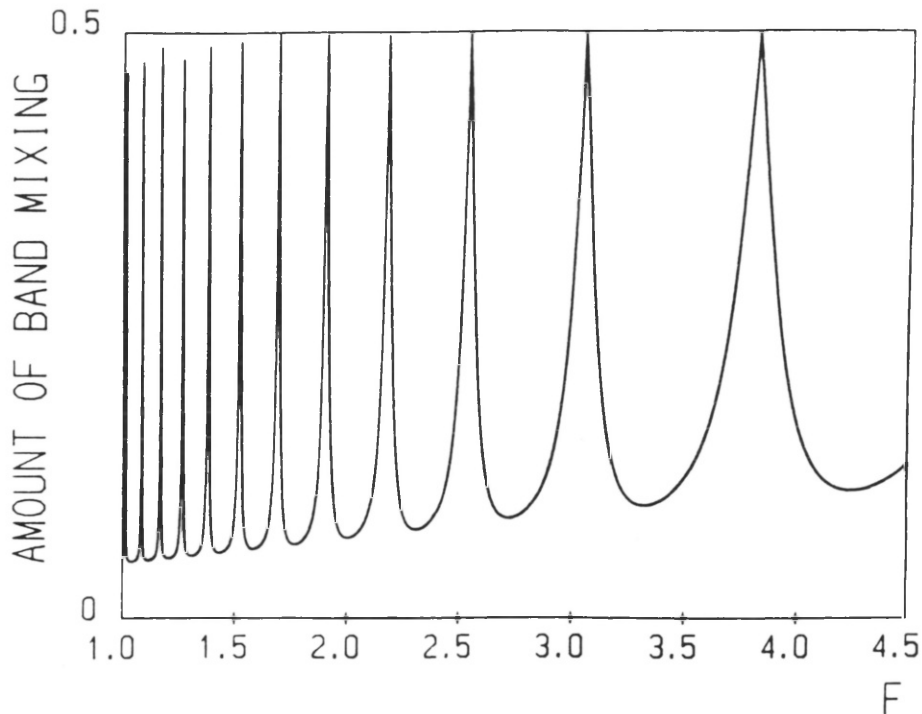


Fig. 5.3 The amount of p state in a wavefunction belonging to the lower band plotted against the electric field.

allowed energy region then its counterpart which points to it having a longer Stark length. Therefore this wavefunction must belong to the wider band (the p-band).

From the way the wavefunctions straddle both bands, it seems evident that there must be tunnelling between the bands at this field and therefore, there must be some mixing of states belonging to different ladders. By varying the field it is possible to vary the relative position of the ladders which must effect the mixing of states belonging to different bands. Furthermore, when the ladders exactly line up and become degenerate with one another, each wavefunction must have an equal component of states belonging to both the s-band and the p-band. Therefore the amount of p-state in a wavefunction belonging to the s-band is plotted against the field (Fig. 5.3) to give an indication of the amount of band mixing at

different fields. Every peak in the graph indicates a degeneracy in energy resulting from the two ladders resonating with each other. This seems to become less frequent however as the field is increased and is certainly not periodic.

The field at which the resonances occur F_r , can be found by using Eq. (4.3). The states in the lower band are labelled as E_n and for the upper band E_m is used. At resonance $E_m = E_n$ which gives

$$F_r = \frac{E_p - E_s}{ea(n-m)} \quad (5.2)$$

where E_p is the zero point of energy for the upper band and E_s is that for the lower band. Resonance between the Stark ladders, therefore, occurs at a field given by the reciprocal of integer numbers ranging from 1 to 49. That is the first resonance occurs when the first Stark state from the p-band ($m=1$) lines up with the 50th Stark states from the s-band ($n=50$). The second resonance will then occur when the second Stark state from the p-band ($m=2$) lines up with the 50th Stark states from the s-band ($n=50$). This is equivalent to the first Stark state from the p-band ($m=1$) lining up with the 49th Stark state from the s-band ($n=49$).

For a one band model Saitoh (1972) derived Eq. (4.10) to give the zero point energy, which for the tight-binding model is $E_p - E_s = \epsilon_p - \epsilon_s$ as the integral of $\cos ka$ ($\epsilon\{k\} = \epsilon - 2V\cos ka$) over the Brillouin zone is zero. Therefore, $E_p - E_s = 14$. By plotting F_r versus $1/(n-m)$ (Fig. 5.4) for the tight-binding model it was found that the points completely lie on a straight line with a gradient of 15.29 ± 0.05 . For $a=e=1$, Eq. (5.2) gives a gradient of 14. This small discrepancy between the two values is due to the fact that the values used for E_p and E_s in Eq. (5.2) are only valid for a one band model. For two interacting bands $E_p - E_s$ can be expected to be somewhat larger.

When the two Stark ladders are in resonance, the

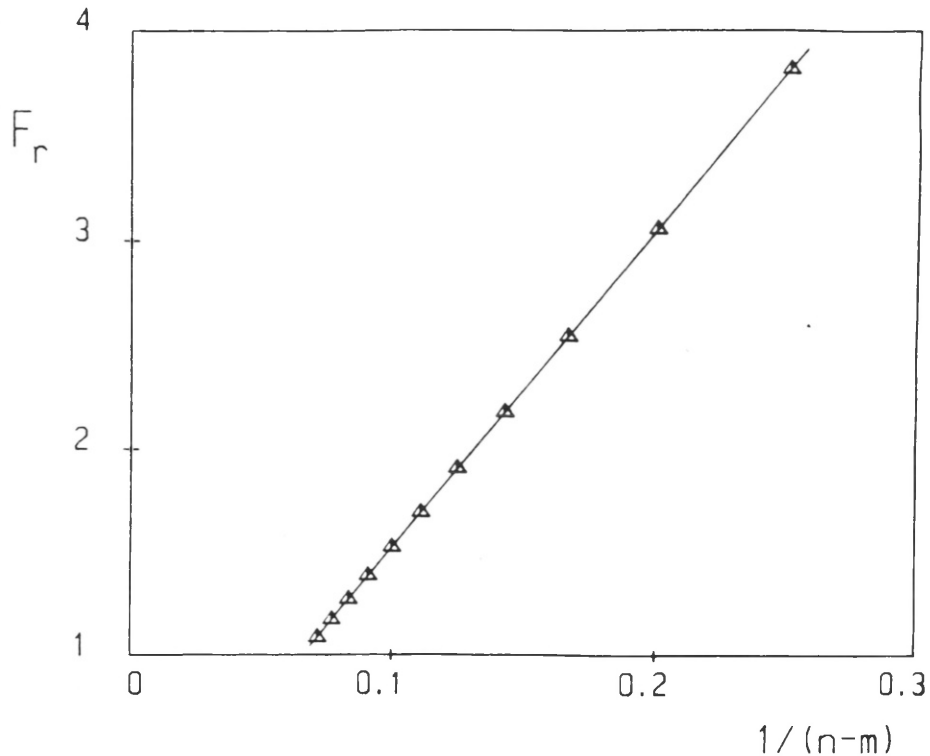


Fig. 5.4 Plot of the electric field at which resonance occurs between the two Stark ladders against the reciprocal of the difference between the indices characterising each Stark state.

Stark-Wannier states in the two bands are degenerate. If there is a non-zero matrix element between the bands then this degeneracy will be lifted and each pair of Stark-Wannier states will split and therefore anticross as the field is varied. In Fig. 5.5 two levels, each one located in different bands, are tracked as the field is varied. If there was a zero matrix element between the bands resulting in a complete absence of Zener tunnelling, then the levels would cross, but it is very clear that they do not cross. This means that if an electron is located in the the lower band, it will cross over to the upper band as the field is varied.

To follow the form of the wavefunction as this happens it is useful to plot the inverse participation ratio P^{-1} which was first introduced by Bell and Dean (1971) in the

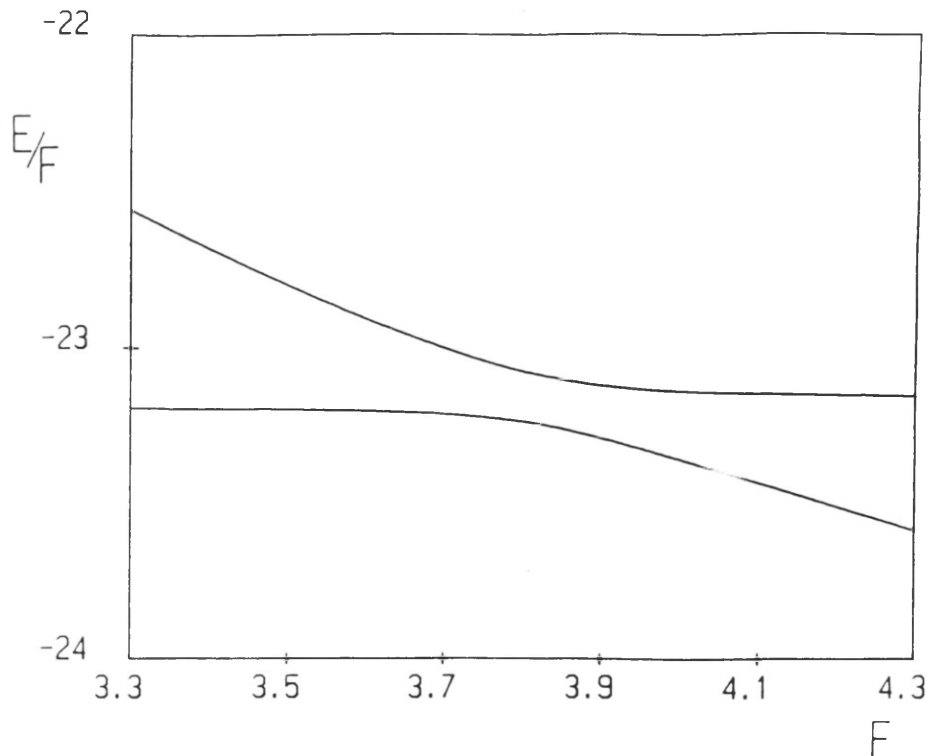


Fig. 5.5 Anticrossing of energy levels belonging to different Stark ladders. This represents a movement of charge between the bands.

theory of localisation. It is defined as

$$P^{-1} = \frac{\sum_i |\Phi_i|^4}{(\sum_i |\Phi_i|^2)^2} \quad (5.3)$$

where Φ_i is the amplitude of the wavefunction on site i . It is effectively a measure of the volume occupied by the wavefunction and can be used as a means of finding the extent of the wavefunction. For example, if it is becoming more extended, P^{-1} will tend to zero as the dominator in Eq.(5.3) dominates over the numerator. However, if the wavefunction is becoming more localised P^{-1} will tend to a constant. Therefore when there is maximum band mixing the wavefunction is at its maximum extension. This is shown in Fig. 5.6. Alignment between the two ladders causes a large

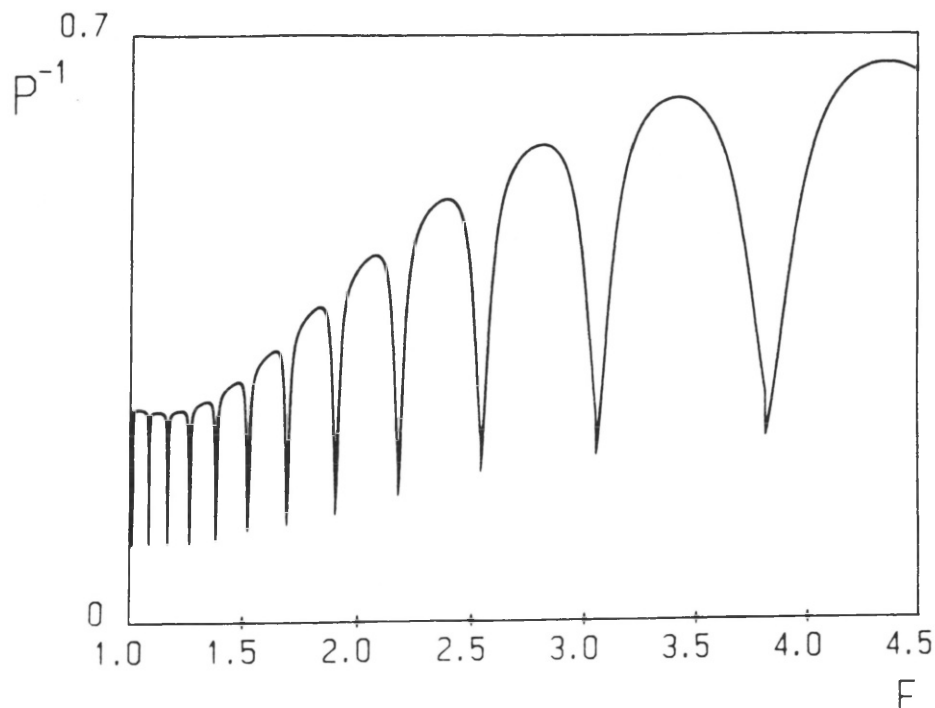


Fig. 5.6 The inverse participation ratio plotted against electric field. Notice that P^{-1} is increasing on average. This is caused by the electrons becoming increasingly localised.

dip in P^{-1} characterising delocalisation. It should also be noted that P^{-1} is getting larger at maximum misalignment as the field is increased. This means that when the wavefunctions are centred on their respective bands, they are becoming more localised. This is in agreement with the fact that the Stark length depends on the inverse of the field ($L_s = W/eF$).

5.4 Zener Tunnelling

The size of the anticrossing of the energy levels can be a useful quantity to know when the size of the tunnel current that is flowing between the two bands is needed. In fact it is a very relevant quantity for characterising

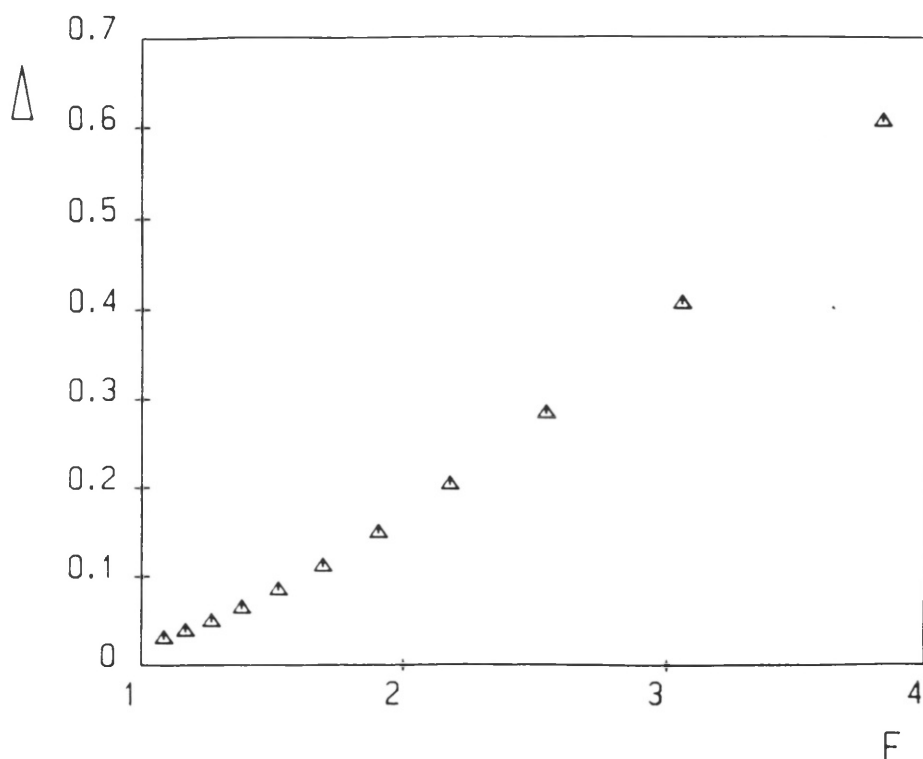


Fig. 5.7 The amount of anticrossing of the two Stark ladders plotted against electric field.

the amount of band mixing. Fig. 5.3 is a useful plot for finding the field at which resonance occurs between the two bands, but it does not convey any information about how strong the resonance is. Consequently, the size of this anticrossing Δ is plotted against the field (Fig. 5.7). Δ clearly increases as the field is increased with the gradient getting steeper as the field gets higher.

It may be argued that the interband coupling is a result of surface effects because a finite system is being considered. However, because an increase in the field results in a decrease in the Stark length, the bulk Stark states interact less with the edges of the sample at larger fields. Therefore, the amount of interband mixing should decrease as the field increases. As this is not observed, it can be concluded that the interband coupling is not a

result of surface effects.

The increase in Δ may be understood in the following way. The distance between the bands, which is given by E_g/eF , is decreasing as the field is increasing. Therefore, the overlap between the two bands is increasing, resulting in a larger splitting of the energy levels. An alternative way of viewing this is that at the lower fields, the two levels that resonate have wavefunctions situated on sites that are fairly widely separated. However, resonances that occur at high fields are between states that are spatially much nearer.

To find a form for Δ as a function of field the following argument is constructed. Using the uncertainty principle the tunnelling time τ is given by

$$\tau \sim \hbar/\Delta \quad (5.4)$$

Therefore the tunnelling rate Γ , which is equal to the reciprocal of the tunnelling time goes as

$$\Gamma \sim \Delta \quad (5.5)$$

At this point an estimate of the tunnelling time between bands can be made. Taking a value for Δ from Fig. 5.7 of 0.2 and translating it into realistic units gives a value of 2meV. This results in a tunnelling time of about 3×10^{-13} s.

From the WKB approximation, the rate Γ is given by

$$\Gamma \sim \exp \left[-2 \int_b^a k \, dx \right] \quad (5.6)$$

where $k^2 = 2m^*/\hbar^2 (V(x) - E)$. From Fig. 4.1, the sloping band gap can be viewed as forming a triangular barrier where

$$V(x) = E_g - eFx \quad (5.7)$$

This gives

$$\Gamma \sim \exp \left[\frac{-4 (2m^*)^{1/2}}{3\hbar} \frac{E_g^{3/2}}{eF} \right] \quad (5.8)$$

Combining (5.8) and (5.5) gives

$$\Delta \sim \exp \left[\frac{-4 (2m^*)^{1/2}}{3\hbar} \frac{E_g^{3/2}}{eF} \right] \quad (5.9)$$

Therefore a plot of $\ln \Delta$ against $1/F$ should result in a straight line of negative gradient. Fig. 5.8 is just such a plot of the data and exhibits a fairly good straight line, especially at lower fields. It is at the higher electric fields where one would expect the above theory to break down. This is because Eq.(5.9) is derived on the assumption that the wavefunctions are plane waves either side of the barrier and that the height of the potential barrier varies slowly in space. Both of these conditions are clearly violated at large electric fields.

It would now seem from this analysis that equations (5.8) and (5.9) do at least give an approximate form for the variation of the rate of tunnelling between the two bands as a function of the field. So instead of having the rather counter-intuitive result that increasing the electric field localises the electrons, as is obtained in the single band picture, it is indeed found that the electric field does increase the current across the sample, albeit only at the points of resonance between the bands. But these resonances are very closely spaced at very low fields and it would not take much broadening attributable to some scattering mechanism to smear all these peaks out.

To observe the resonances, however, it must be ensured that not all of them are broadened out. There are many possible scattering mechanisms which could result in broadening but two of the most likely mechanisms are electron-optic phonon scattering to other Stark states and

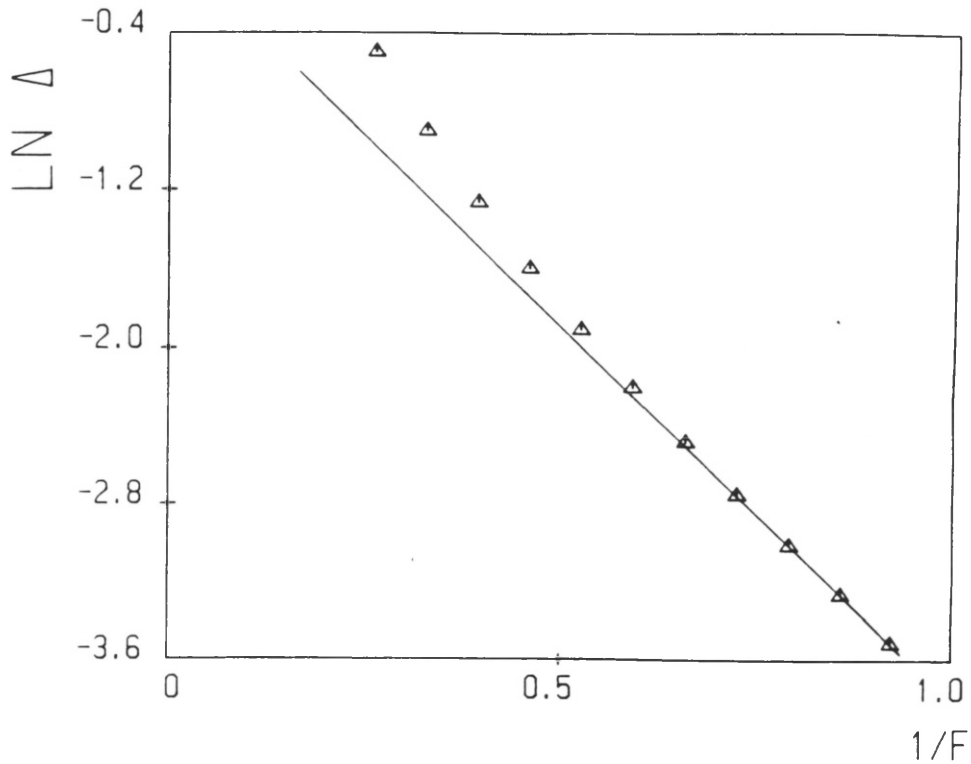


Fig. 5.8 The natural logarithm of the amount of anticrossing of the two Stark ladders plotted against the reciprocal of the electric field.

tunnelling out of the sample and into the contact region. In fact the second of these is essential for any type of current to flow. Therefore, this broadening is unavoidable. For Lorentzian broadening the profile of the resonance is given by

$$\frac{(\Gamma/2)^2}{(E-E_r)^2 + (\Gamma/2)^2} \quad (5.10)$$

where E_r is the position of the resonance and Γ is the full width at half maximum and is given by the lifetime of the Stark-Wannier states. For electron-optic phonon interactions the scattering time is approximately 1×10^{-13} s which results in a Γ_{e-p} of 6 meV. To make an estimate of the rate of tunnelling into the contact region, it is

assumed that this is of the same order of magnitude as the tunnelling rate between bands, therefore $\Gamma_{\text{con}} \sim 2\text{meV}$. These amounts of broadening, therefore, still make it possible to observe at least some of the resonances, especially at high fields when they can be spaced at intervals of about 0.5eV . In fact in chapter 8 the transfer matrix method, which explicitly includes the coupling to other states, is used to look at these resonances and it is found that they are indeed observable.

Because a tight-binding model is being studied, the field has no effect on the individual sites. Therefore, in the language of Emin and Hart (1987), effectively only the Step function potential in the Hamiltonian is being considered and this should give no interband coupling. However, it has been shown that interband mixing is obtained using this model. To investigate this, the interband matrix element $\langle n, k | x | n', k' \rangle$ for the two band tight-binding model of finite length will now be studied. The basis functions $|n, k\rangle$ are now given by

$$|n, k\rangle = e^{ikpa} [S_{n,k} |s\rangle + P_{n,k} |p\rangle] \quad (5.11)$$

on each site. S is the s-like function and P is the p-like function which both depend on the wavevector k and the band index n . Following Emin and Hart, the x in the matrix element is replaced by the Step function

$$\begin{aligned} S(x) &= 0 \quad \text{for } x < 1 \\ S(x) &= 1 \quad \text{for } x \geq 1 \end{aligned} \quad (5.12)$$

to give

$$\begin{aligned} &\langle n, k | \sum_{m=1}^N S(x/a-m) | n', k' \rangle \\ &= \int_0^{Na} [\langle s | S_{n,k}^* + \langle p | P_{n,k}^*] \sum_{m=1}^N S(x/a-m) [S_{n',k'} |s\rangle + P_{n',k'} |p\rangle] \\ &\quad \times e^{i(k'-k)pa} dx \end{aligned}$$

$$\begin{aligned}
&= \sum_{p=1}^N p e^{i(k'-k)pa} \int_0^a [\langle s | S_{n,k}^* + \langle p | P_{n,k}^*] [S_{n',k'} | s \rangle + P_{n',k'} | p \rangle] dx \\
&= -i \frac{N}{a} \frac{\partial}{\partial k'} \left[\delta_{k,k'} \right] I(n,k;n',k') \quad (5.13)
\end{aligned}$$

Again use has been made of the relation given in Eq.(4.12). Eq.(5.13), not surprisingly, has the same form as the second term in Eq.(4.14), but with a different $I(n,k;n',k')$. This is now substituted back into the Schrödinger equation given in Eq.(4.5) to obtain

$$\begin{aligned}
[\varepsilon(n,k) - E] C(n,k) &= -ieFN \sum_{n',k'} \frac{\partial}{\partial k'} \left[\delta_{k,k'} \right] I(n,k;n',k') C(n',k') \\
&= ieFN \sum_{n',k'} \delta_{k,k'} \frac{\partial}{\partial k'} \left[I(n,k;n',k') C(n',k') \right] \\
&= ieFN \left[\frac{\partial}{\partial k} C(n,k) + \right. \\
&\quad \left. \sum_{n',k'} \delta_{k,k'} C(n',k') \frac{\partial}{\partial k'} I(n,k;n',k') \right] \quad (5.14)
\end{aligned}$$

where the relation (Emin and Hart 1987)

$$\delta_{k,k'} I(n,k;n',k') = \delta_{n,n'} \delta_{k,k'} \quad (5.15)$$

is used to obtain the first term in Eq.(5.14) above. The following relation has also been used

$$\sum_{k'} \frac{\partial}{\partial k'} \left[I(n,k;n',k') C(n',k') \delta_{k,k'} \right] = 0 \quad (5.16)$$

This relation is valid because the function being differentiated is a periodic function of k' . It is also quite justified to have a discrete set of k' 's and a continuous derivative in Eq.(5.16). This point is shown to be true in Appendix A for a general periodic function of

k' . The derivative of $I(n, k; n', k')$ with respect to k' can be written

$$\delta_{k, k'} \frac{\partial}{\partial k'} I(n, k; n', k') = \delta_{k, k'} \int_0^a [\langle s | S_{n, k}^* + \langle p | P_{n, k}^*] \frac{\partial}{\partial k'} [S_{n', k'} | s \rangle + P_{n', k'} | p \rangle] dx \quad (5.17)$$

This is the important term which couples the bands and cannot be zero unless the S and P functions are independent of k . This is because $[S_{n', k} | s \rangle + P_{n', k} | p \rangle]$ is orthonormal to $[S_{n, k} | s \rangle + P_{n, k} | p \rangle]$ for $n \neq n'$. Therefore these can be viewed as two perpendicular vectors in a two dimensional space lying on a unit circle. Consequently, the derivative with respect to k of $[S_{n', k} | s \rangle + P_{n', k} | p \rangle]$ must lie parallel to $[S_{n, k} | s \rangle + P_{n, k} | p \rangle]$ which means the right hand side of Eq.(5.17) is non-zero. The only way it could be zero is if the bands were decoupled in the first place which would mean that effectively a single band model was being studied. There is in fact an error in Emin and Hart's paper which results in the right hand side of Eq.(5.17) being zero. This is explained in Appendix B at the end of this chapter.

5.5 Multiband Stark-Wannier States

This section will now concentrate on the actual form of the Stark-Wannier states. This will allow a comparison to be made with the one obtained analytically by Saitoh in the single band model (Eq.(4.9)). Fig. 5.9 is a plot of the Stark-Wannier wavefunctions when the two bands are at resonance (i.e. the two wavefunctions represent the two energy states given in Fig. 5.5 when they are at maximum anticrossing). It is clear from this plot that the resultant wavefunctions are linear combinations of two states, each one centred on and belonging to a different

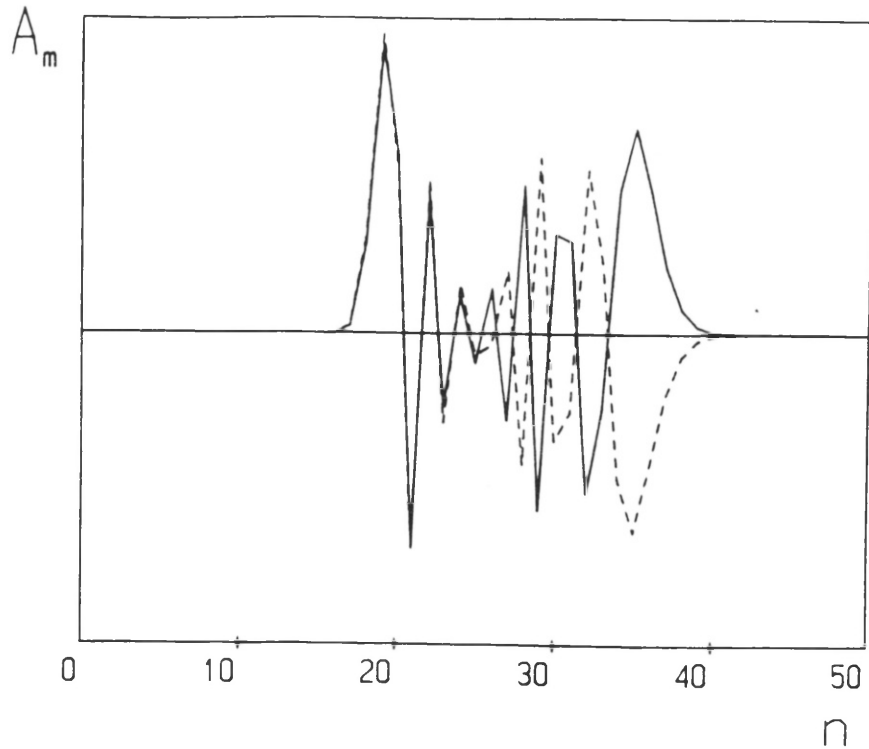


Fig. 5.9 Two Stark-Wannier wavefunctions plotted at resonance. The wavefunctions seem to be superpositions of the single band states.

band. The wavefunction represented by a continuous line, $A_m^1(x)$ is therefore given by

$$A_m^1(x) = |1\rangle + |2\rangle \quad (5.18)$$

whilst $A_m^2(x)$ which is represented by the dashed line is given by

$$A_m^2(x) = |1\rangle - |2\rangle \quad (5.19)$$

The form for the states $|1\rangle$ and $|2\rangle$ closely resemble the Bessel function solutions for the single band case. It is therefore concluded that the Stark-Wannier states for a multiple band system are simply a superposition of the single band states which are Bessel functions of the first

kind.

5.6 Conclusion

It was mentioned in the last chapter that superlattices are good for forming Stark ladders because the large fields that are attainable and the narrow band widths result in a Stark length much shorter than the length of the sample. However, to observe the aperiodic Zener oscillations described in this chapter, the sample must be longer than a 'Super' Stark length calculated using both the valence and conduction bands and the gap that separates them.

e.g.

$$L > W_1/eF + E_g/eF + W_2/eF \quad (5.20)$$

where L is the length of the sample, W_1 is the valence band width, E_g is the energy gap and W_2 is the conduction band width. Using the band widths and gaps quoted in the last chapter from the paper by Esaki and Chang, an effective band width of 0.25eV is obtained. If the superlattice is say 50 periods long, then to observe Zener tunnelling the Stark length must be less than 0.45 μ m. This can be obtained with a field strength of 5.5x10³V/cm.

Measuring the V-I characteristics of a superlattice may not, however, be the best way to observe the Stark states. A very powerful and more sensitive method is optical absorption. This will be treated in the next chapter.

Appendix A

To illustrate that Eq.(5.16) is meaningful, consider any periodic function of k . This function can be written as the following Fourier series

$$\sum_{m=-\infty}^{\infty} e^{ikma} C_m \quad (A1)$$

The derivative of this function is now taken with respect to k to give

$$\frac{\partial}{\partial k} \left[\sum_{m=-\infty}^{\infty} e^{ikma} C_m \right] = \sum_{m=-\infty}^{\infty} i m a e^{ikma} C_m \quad (A2)$$

As a finite system is being considered, only values of k that are integer multiples of $2\pi/Na$ (where Na is the length of the system) are allowed. Therefore restricting k to these values in (A2) and summing over k gives

$$\begin{aligned} \sum_k \sum_{m=-\infty}^{\infty} i m a e^{ikma} C_m &= \sum_{n=0}^{N-1} \sum_{m=-\infty}^{\infty} i m a e^{i(2\pi/Na)nma} C_m \\ &= \sum_{m=-\infty}^{\infty} i m a \sum_{n=0}^{N-1} e^{i(2\pi/Na)nma} C_m \end{aligned} \quad (A3)$$

The sum over n is the Kronecker delta given in Eq.(4.12). Therefore this term is zero unless $m=0$. If $m=0$ then the whole of the right hand side of Eq.(A3) is zero. Therefore the sum over k of the derivative of the periodic function is zero, even if k is discrete.

Appendix B

In the paper by Emin and Hart, they showed that the term in the Schrödinger equation that couples different bands under the influence of an electric field results from the alteration of the shape of the potential wells. The numerical work in this chapter has shown that this cannot be correct because by using the tight-binding model any field dependent alteration of the potential wells is neglected which means a Step function potential is effectively being considered. In spite of this, band coupling is still observed. Using Eqs. (5.14) and (5.17) it has been shown that the only way the bands could possibly be decoupled when there is a field present is if they were decoupled in the unperturbed system. Therefore, there must be a mistake in Emin and Hart's paper that leads them to their conclusion.

From Eq. (5.17)

$$\delta_{k,k'} \frac{\partial}{\partial k'} I(n,k;n',k') = \delta_{k,k'} \int_0^a [\langle s | S_{n,k}^* + \langle p | P_{n,k}^*] \frac{\partial}{\partial k'} [S_{n',k'} | s \rangle + P_{n',k'} | p \rangle] dx \quad (B1)$$

cannot be zero. In Emin and Hart's paper they prove in the appendix that this is indeed zero. However, during the proof they make a serious mistake. They are trying to show that the derivative of $\delta_{n,n'} \delta_{k,k'}$ with respect to k' at $k=k'$ is $\delta_{n,n'} \delta_{k,k'} a(N-1)/2$. They do this by writing the two delta functions in terms of Wannier functions. However, they use the orthogonality relation

$$\int_0^{Na} w_n^*(x-pa) w_{n'}(x-p'a) dx = \delta_{n,n'} \delta_{p,p'} \quad (B2)$$

where $w(x-pa)$ is the Wannier function centred on $x=pa$ and the integral is over the whole system. However, (B2) is incorrect. The Wannier functions are only orthogonal in this way if the integral is from minus infinity to

infinity. The problem is that the Wannier functions located at the edge of the system are not orthogonal to the bulk Wannier functions. There is, therefore, an extra surface term which has been neglected in Emin and Hart's paper and which when included no longer results in (B1) being zero.

The derivative of $\delta_{n,n'}\delta_{k,k'}$ with respect to k' at $k=k'$ will now be calculated to show that in addition to $\delta_{n,n'}\delta_{k,k'}a(N-1)/2$, the derivative of $I(n,k;n',k')$ with respect to k' is obtained. This is performed by replacing the delta functions by two orthogonal Bloch functions, therefore

$$\left. \frac{\partial}{\partial k'} (\delta_{n,n'}\delta_{k,k'}) \right|_{k=k'} = \frac{\partial}{\partial k'} \left[\frac{1}{N} \int_0^{Na} e^{i(k'-k)x} u_{nk}^*(x) u_{n',k'}(x) dx \right]_{k=k'} \quad (B3)$$

These Bloch functions could be the field dependent type derived in Emin and Hart's paper. The integral is then reduced to a unit cell to give

$$\begin{aligned} & \left. \frac{\partial}{\partial k'} \left[\frac{1}{N} \sum_{p=0}^{N-1} e^{i(k'-k)pa} \int_0^a e^{i(k'-k)x} u_{nk}^*(x) u_{n',k'}(x) dx \right] \right|_{k=k'} \\ &= \frac{1}{N} \sum_{p=0}^{N-1} i a p e^{i(k'-k)pa} \int_0^a e^{i(k'-k)x} u_{nk}^*(x) u_{n',k'}(x) dx \Big|_{k=k'} \\ &+ \frac{1}{N} \sum_{p=0}^{N-1} e^{i(k'-k)pa} \frac{\partial}{\partial k'} \int_0^a e^{i(k'-k)x} u_{nk}^*(x) u_{n',k'}(x) dx \Big|_{k=k'} \end{aligned}$$

$$\begin{aligned}
&= \frac{1}{N} \sum_{p=0}^{N-1} i a p \int_0^a u_{nk}^*(x) u_{n',k}(x) dx \\
&\quad + \delta_{k,k'} \frac{\partial}{\partial k'} \int_0^a e^{i(k'-k)x} u_{nk}^*(x) u_{n',k'}(x) dx \\
&= \frac{(N-1)}{2} i a \delta_{n,n'} \delta_{k,k'} + \delta_{k,k'} \frac{\partial}{\partial k'} I(n,k;n',k') \quad (B4)
\end{aligned}$$

Therefore the extra term that was absent in Emin and Hart's result has now been regained. Also note that the second term cannot simply be cancelled in the limit N goes to infinity even though it is a surface term. In the next step in Emin and Hart's argument another quantity is calculated which involves the same term of order $(N-1)$ as in Eq.(B4). These terms are then subtracted to yield a result of order unity. Therefore, the limit of N tending to infinity has to be taken after this subtraction to leave a term of finite proportions.

6 OPTICAL ABSORPTION IN A BIASED SUPERLATTICE

6.1 Introduction

Gaining knowledge about the electronic structure of MQWs and superlattices by measuring their transport characteristics can be termed 'tunnelling spectroscopy'. However, this technique still suffers from a few drawbacks which makes spectroscopy using light more practical in certain circumstances.

For instance, in the last chapter it was shown that the indirect observation of Stark states can be achieved via the observation of the aperiodic Zener resonances in the current where the field at which the resonances occur show that the states do indeed lie on a Stark ladder. However, the actual experimental observation of these resonances could prove extremely difficult. For example, it has already been mentioned that the movement of electrons through the sample can produce high field domains which would destroy the Stark ladder. Also if the coupling between the states or between the states and the edges is fairly strong, then the resonances could be very weak and might not be observable. Conversely, if the Stark states are very weakly coupled, then the current that is allowed to flow through the sample may be too small to allow for the observation of the resonances. However, even in the light spectroscopy case there could be some spectral broadening caused by the escape of photoexcited electrons from the Stark states. This though would probably be a fairly small effect (i.e. see Levine et al 1988).

Therefore, it makes sense to investigate transitions that may occur between the Stark states when the sample is exposed to electromagnetic radiation. This may also have consequences for the construction of an infrared detector (Choi et al 1987b, 1987c and 1988, Levine et al 1987a and Liu et al 1988). Furthermore, as the transport properties of the device are not being measured directly, there is no need for a current to flow. Therefore, much higher electric fields can be generated without resulting in electrical breakdown. This of course makes the observation of field induced effects like Stark states and Stark localisation much more achievable.

Mendez and co-workers (1988) have already performed an experiment related to this work that has really revealed the benefit of using light spectroscopy. By applying a bias across a superlattice to form a Stark ladder, they were able to photoexcite carriers from the hole band into the electron band (see Fig. 6.1) thus allowing the localising properties of the Stark states to be unambiguously observed. Other similar experiments have included the investigation of transitions between the states of an unbiased single quantum well (Seilmair et al 1987 and Kane et al 1988).

In this chapter optical absorption taking place between Stark states located in different bands and between a Stark state and the continuum will be investigated for a superlattice in the presence of a constant electric field. Experimentally, this particular case has not been investigated, although Levine et al (1987b) have studied a 50 period GaAs/AlGaAs superlattice under a bias. However, this structure did not have a uniform electric field dropped across it, instead the high field domains mentioned in chapter 4 were present because a current was allowed to flow. The optical transitions that were observed, therefore, were not between Stark states but were between the individual quantum well states.

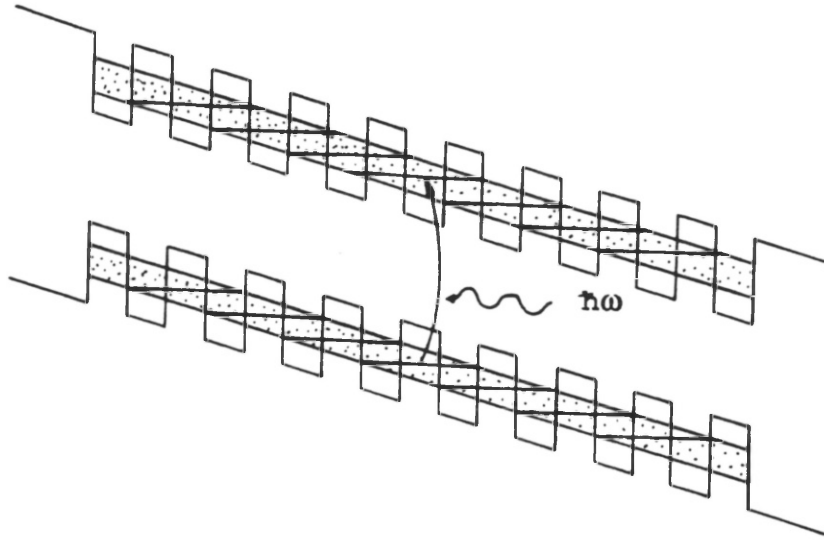


Fig. 6.1 The conduction and valence band potential profiles for a superlattice in the presence of a high electric field. Only one miniband is formed in each set of wells. The optical transition between Stark states in each miniband is shown.

6.2 Direct Optical Transitions

Consider the following Hamiltonian for a superlattice in the presence of a static electric field and a source of electromagnetic radiation

$$H = \frac{(\underline{p} + e\underline{A})^2}{2m^*} + V(\underline{r}) - eFx \quad (6.1)$$

By comparing this with Eq.(4.1) it can be seen that the radiation has induced a change of momentum given by

$$\underline{p} \rightarrow \underline{p} + e\underline{A} \quad (6.2)$$

where $\underline{A}$ is the vector potential characterising the electromagnetic field and for a monochromatic source can be

written

$$\underline{A} = A_0 \underline{\varepsilon} e^{i(\underline{q} \cdot \underline{r} - \omega t)} \quad (6.3)$$

where $\underline{\varepsilon}$ is the polarisation vector. The Hamiltonian (6.1) can be written

$$H = H_0 + H' \quad (6.4)$$

where H' is the perturbation due to the photon and is given by

$$H' = (e/m^*) \underline{p} \cdot \underline{A} \quad (6.5)$$

The $\underline{A}^2$ term has been neglected and a suitable gauge has been selected so that $\text{div } \underline{A} = 0$.

The absorption coefficient for optically induced transitions is given by (Madelung 1981)

$$K = \frac{2\pi}{\varepsilon_0 n e \omega A_0^2} W \quad (6.6)$$

where n is the refractive index and W is the following transition rate

$$W = \frac{2\pi}{\hbar} |\langle j'k' | H' | jk \rangle|^2 \delta(E_{j'} + \hbar\omega - E_j) \quad (6.7)$$

where $|jk\rangle$ and $|j'k'\rangle$ are the initial and final states respectively, k and k' are momenta characterising these states and H' is the perturbation given above. The matrix element in (6.7) can be written

$$\begin{aligned} \langle j'k' | H' | jk \rangle &= \frac{-i\hbar e}{m} \langle j'k' | \underline{A} \cdot \underline{\nabla} | jk \rangle \\ &= \frac{-i\hbar e}{m} A_0 \langle j'k' | e^{i\underline{q} \cdot \underline{r}} \underline{\varepsilon} \cdot \underline{\nabla} | jk \rangle e^{-i\omega t} \end{aligned} \quad (6.8)$$

By momentum conservation $k+q=k'$. However the change of electron momentum is small because the q -vector is several orders of magnitude less than the Brillouin zone. Therefore to a good approximation $q=0$ and $k=k'$.

As optical transitions between one dimensional Stark states (i.e. states that are only x -dependent) are being considered, maximum absorption is achieved when the polarisation of the incident wave is parallel to the x -direction (i.e. the direction of the superlattice period). By considering just this one dimension, the rate W can be written

$$\langle j' | H' | j \rangle = \frac{-i\hbar e}{m} A_0 \langle j' | \frac{\partial}{\partial x} | j \rangle e^{-i\omega t} \quad (6.9)$$

By using the equation of motion for x

$$i\hbar \frac{dx}{dt} = [x, H] \quad (6.10)$$

the derivative above in (6.9) can be replaced by $m\omega x/\hbar$. Therefore

$$\langle j' | H' | j \rangle = -i\omega e A_0 \langle j' | x | j \rangle e^{-i\omega t} \quad (6.11)$$

The absorption coefficient can now be written

$$\kappa = \frac{4\pi\omega e}{\epsilon_0 n} |\langle j' | x | j \rangle|^2 \delta(E_j + \hbar\omega - E_{j'}) \quad (6.12)$$

6.3 The Stark-Stark Transition

The transition between two single band Stark-Wannier states, one localised in the conduction band and one localised in the valence band will now be considered. This is a very similar situation to that shown in Fig. 6.1 except that both the bands are now formed by the top set of

quantum wells. The valence band wavefunction can be written (4.9)

$$S_v(x) = \frac{\sqrt{a}}{2\pi} \int_{-\pi/a}^{\pi/a} e^{ikx-i(W/2eFa)\sin ak} dk \quad (6.13)$$

where this wavefunction is centred on the origin with energy ϵ_v . However, as transitions between different bands are being considered, the actual differences between the states that make up the bands must be included explicitly to avoid any selection rules that may arise resulting from the symmetry between the two bands. Therefore, the tight-binding approximation is used to give

$$S_v(x) = \frac{\sqrt{a}}{2\pi} \int_{-\pi/a}^{\pi/a} \sum_n e^{ikna-i(W/2eFa)\sin ak} \Phi_v(x-na) dk \quad (6.14)$$

And similarly for the conduction band Stark wavefunction

$$S_c(x) = \frac{\sqrt{a}}{2\pi} \int_{-\pi/a}^{\pi/a} \sum_{n'} e^{ipna-imap+i(V/2eFa)\sin ap} \Phi_c(x-na) dp \quad (6.15)$$

where this wavefunction is centred on $x=ma$ with energy ϵ_c+eFam and V is now the band width. The Φ 's are the quantum well states and are given by

$$\Phi_v(x) = \begin{cases} \sqrt{(2/L)} \cos(\pi x/L) & |x| \leq L/2 \\ 0 & L/2 \leq |x| \leq a-L/2 \end{cases} \quad (6.16)$$

$$\Phi_c(x) = \begin{cases} \sqrt{(2/L)} \sin(2\pi x/L) & |x| \leq L/2 \\ 0 & L/2 \leq |x| \leq a-L/2 \end{cases} \quad (6.17)$$

where L is the width of the quantum wells.

To facilitate the evaluation of the matrix element in

(6.12) the following trick is used.

$$\langle S_C | x | S_V \rangle = \lim_{q \rightarrow 0} \frac{1}{i} \frac{\partial}{\partial q} \langle S_C | e^{iqx} | S_V \rangle \quad (6.18)$$

Substituting (6.14) and (6.15) into this and performing the p and x integration and the sums over n and n' gives

$$\begin{aligned} \langle S_C | e^{iqx} | S_V \rangle = & \\ \frac{i\sqrt{a}}{\pi L} \int_{-\pi/a}^{\pi/a} \exp \left[-i(V/2eFa) \sin a(k+q) - i(W/2eFa) \sin ak + ima(k+q) \right] & \\ \times q \cos(qL/2) \left[\frac{1}{q^2 + \pi^2/L^2} - \frac{1}{q^2 + 9\pi^2/L^2} \right] dk & \quad (6.19) \end{aligned}$$

Differentiating with respect to q and taking the limit that q tends to zero gives

$$\langle S_C | x | S_V \rangle = \frac{16}{9} \frac{L}{\pi^2} J_m'([V+W]/2eFa) \quad (6.20)$$

where J_m is the Bessel function. Therefore the absorption coefficient is given by

$$\kappa = \frac{4\pi\omega e}{\epsilon_0 n} \frac{1024}{81} \frac{L^2}{\pi^3} |J_m'([V+W]/2eFa)|^2 \delta(E_V + \hbar\omega - E_C) \quad (6.21)$$

with the energy conserving delta function requiring

$$m = \frac{\hbar\omega - (\epsilon_C - \epsilon_V)}{eFa} \quad (6.22)$$

Therefore only photons with an energy that matches the energy difference between two Stark states can be absorbed. Fig.6.2 is a plot of the envelope of the absorption lines given by Eq.(6.21) as a function of photon energy with a sum over the final states at $F=2 \times 10^5 \text{Vm}^{-1}$. The band widths, W and V, were set at 0.01eV and 0.05eV respectively, the energy gap to 0.25eV and the lattice constant to 10^{-8}m . The rapid decay of the envelope either side

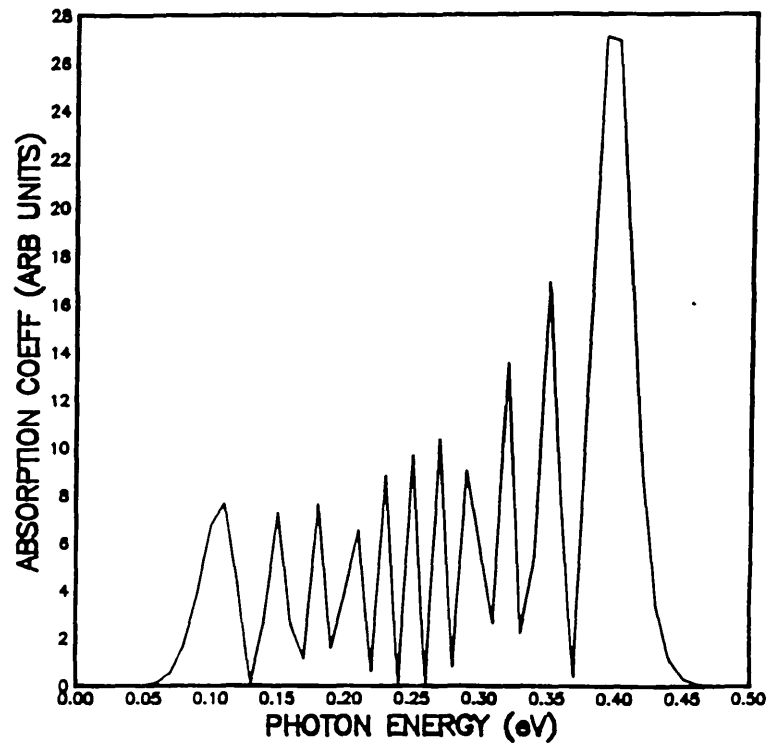


Fig. 6.2 The envelope of the optical absorption coefficient as a function of incident photon energy at a field of $2 \times 10^5 \text{ Vm}^{-1}$ for a transition between Stark states located in different bands.

of the main central feature is caused by the very small overlap that exists between Bessel functions that are fairly widely separated. In fact the decay of the Bessel function is given by

$$J_n^2(x) \sim 1/\pi x_n (x/x_n)^{2n} \quad (6.23)$$

for $x_n > x$ and where $x_n \sim n$. This means that when the wavefunction is outside the Stark length (i.e. outside the confines of the band) the wavefunction decays very rapidly indeed. Therefore, for there to be a non-zero absorption coefficient, there must be significant overlap between the Stark lengths of the two states being considered.

Fig. 6.3 shows the envelope of the absorption coefficient at a slightly higher field of $F = 6 \times 10^5 \text{ Vm}^{-1}$. As might be

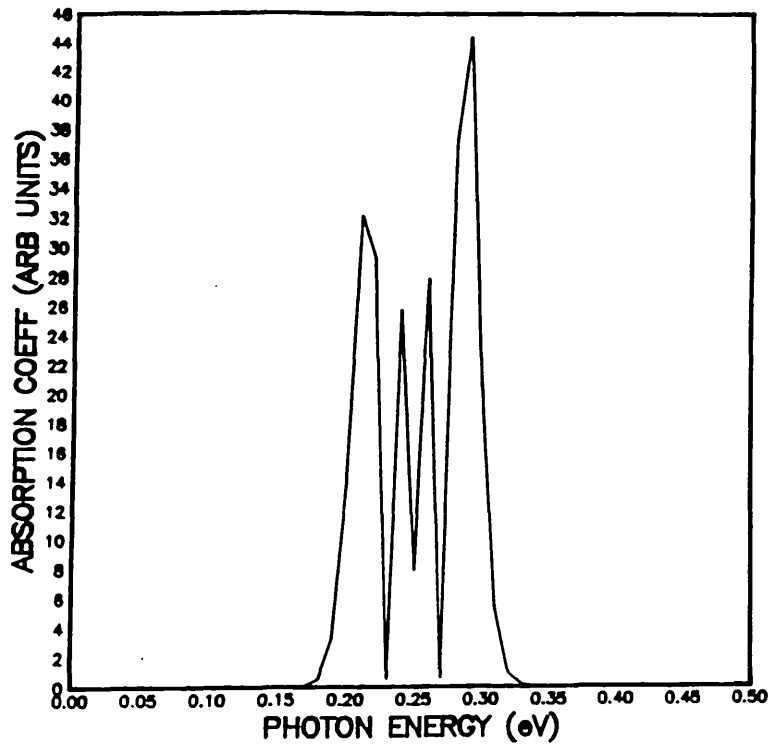


Fig. 6.3 The envelope of the optical absorption coefficient as a function of incident photon energy at a field of $6 \times 10^5 \text{ Vm}^{-1}$ for a transition between Stark states located in different bands.

expected, the graph becomes more localised as the Stark length of each wavefunction becomes shorter thus reducing the amount of overlap between states.

However, these graphs would not be expected to be observed experimentally. This is because broadening, caused by the electrons tunnelling out of the Stark states, smears out the spiky structure. To simulate the absorption coefficient more realistically the delta function in Eq.(6.21) is replaced by the Lorentzian

$$\frac{(\Gamma/2)^2}{(\Gamma/2)^2 + (E_v + \hbar\omega - E_c)^2} \quad (6.24)$$

where Γ is the full width a half maximum of the broadened peak. Fig. 6.4 and Fig. 6.5 display the absorption

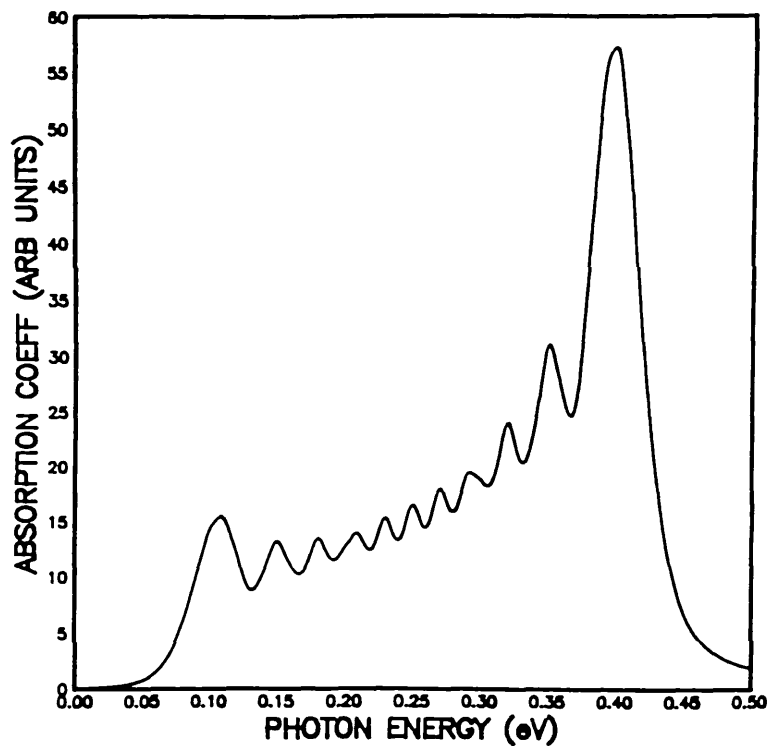


Fig. 6.4 The Lorentzian broadened optical absorption rate as a function of incident photon energy at a field of $2 \times 10^5 \text{ Vm}^{-1}$ for a transition between Stark states located in different bands.

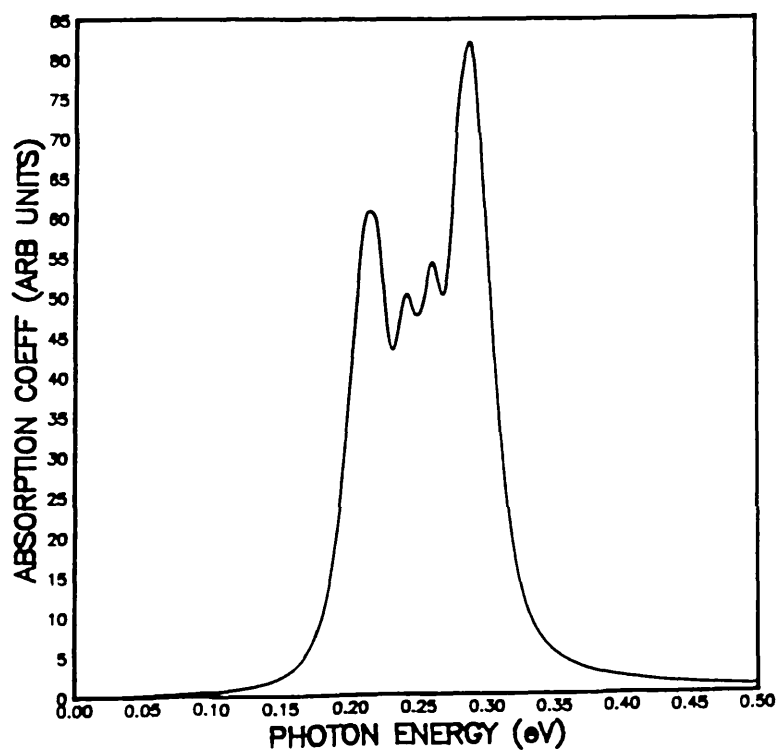


Fig. 6.5 The Lorentzian broadened optical absorption rate as a function of incident photon energy at a field of $6 \times 10^5 \text{ Vm}^{-1}$ for a transition between Stark states located in different bands.

coefficient with the above broadening at $F=2 \times 10^5 \text{Vm}^{-1}$ and $F=6 \times 10^5 \text{Vm}^{-1}$ respectively. These graphs both show the smoothing out of the spiky structure into something which would be expected to be observed experimentally.

6.4 The Stark-Airy Transition

It is also possible for the incoming electromagnetic radiation to cause transitions between the Stark states and the continuum above the bands (it should be noted here, as in chapter 2, that there may be small gaps in the energy region above the bands, but these will be ignored and it will be assumed that a continuum exists above the bands). It was shown in chapter 2 (section 2.3) that in an electric field these states are described by Airy functions and can be written

$$A(x) = \frac{1}{\pi} \int_0^{\infty} \cos \left[s^3/3 - sA'(x + [E - \Delta]/e\hbar) \right] ds \quad (6.25)$$

where $A' = (2m^* eF/\hbar^2)^{1/3}$ and Δ is the energy of the Airy function which changes from its oscillatory solution to its decaying form at $x=0$ (see Fig. 6.6). The Stark state is centred on $x=0$ and as before is written

$$S_c(x) = \frac{\sqrt{a}}{2\pi} \int_{-\pi/a}^{\pi/a} \sum_n e^{ikna + i(V/2eFa) \sin ak} \Phi_c(x - na) dk \quad (6.26)$$

Again the x in the matrix element is replaced by e^{iqx} and now with the Airy and Stark wavefunctions can be written (after summing over n)

$$\begin{aligned} \langle A | e^{iqx} | S_c \rangle = & \frac{\sqrt{a}}{2\pi} \int_{-\pi/a}^{\pi/a} \exp \left[-i(k+q)^3/A'^3 - iE(k+q) + i(V/2eFa) \sin ak \right] \\ & \times \sqrt{(2/L)} \cos(kL/2) \left[\frac{2\pi/L}{k^2 + \pi^2/L^2} \right] dk \quad (6.27) \end{aligned}$$

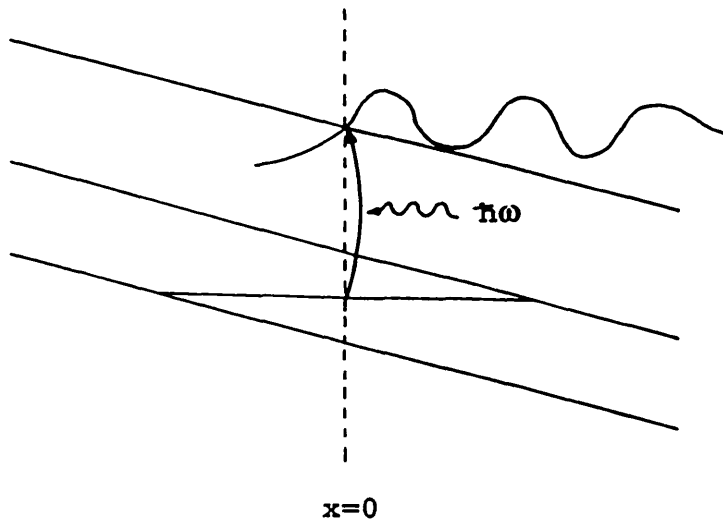


Fig. 6.6 Sketch showing an optical transition between a Stark state and an Airy-Continuum state. The Airy wavefunction changes from its oscillatory form to its decaying state at $x=0$.

Differentiating with respect to q and taking the limit $q \rightarrow 0$ gives

$$\langle A | e^{iqx} | S_c \rangle = \frac{\sqrt{a}}{\pi} \int_0^{\pi/a} \cos(k^3/\dot{A}^3 - Ek + \{V/2eFa\} \sin ka) \times [3k^2/\dot{A}^2 - E] \cdot \cos(kL/2) \cdot 1/[k^2 + \pi^2/L^2] dk \quad (6.28)$$

Therefore, the absorption coefficient for an optically induced direct transition between a Stark state and an continuum Airy wavefunction is

$$K = \frac{4\pi\omega e}{\epsilon_0 m} \left[\frac{\sqrt{a}}{\pi} \int_0^{\pi/a} [3k^2/\dot{A}^2 - E] \cdot \cos(kL/2) \cdot 1/[k^2 + \pi^2/L^2] \times \cos(k^3/\dot{A}^3 - Ek + \{V/2eFa\} \sin ka) dk \right]^2 \delta(E_c + \hbar\omega - E) \quad (6.29)$$

Because the Airy states are not quantised like the

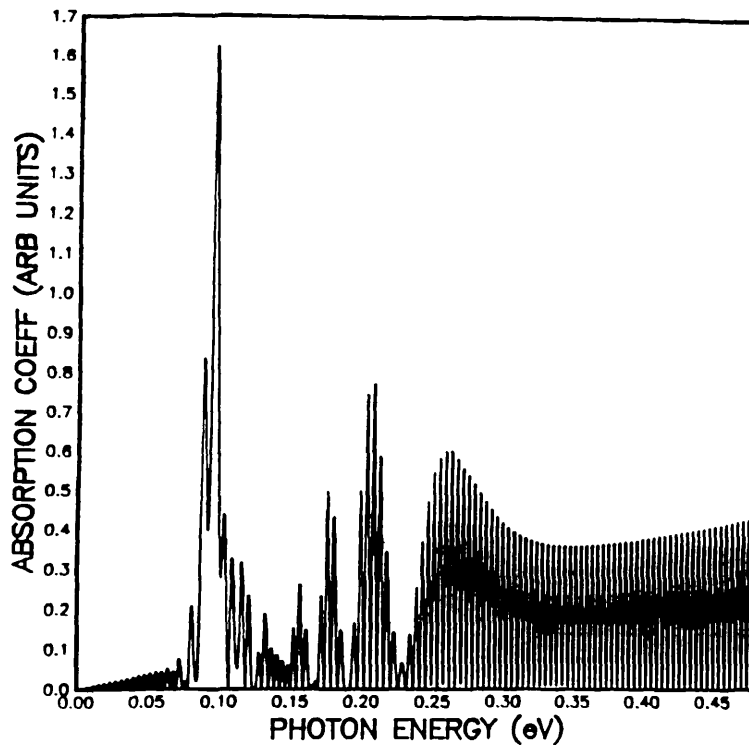


Fig. 6.7 The optical absorption rate between a Stark state and an Airy-Continuum state as a function of incident photon energy at a field of 10^6 Vm^{-1} .

Stark states, the delta function can be satisfied for any photon energy.

To find the form of the absorption coefficient above, the integral has to be evaluated numerically. Fig. 6.7 displays the absorption coefficient at $F=10^6 \text{ Vm}^{-1}$. For this calculation $V=0.05 \text{ eV}$, the gap between the band and the continuum was 0.1 eV , $m^*=0.067m_0$ and again $a=10^{-8} \text{ m}$. The striking difference between this and the Stark-Stark transition is that the photon energy can be as large as one requires and still give a finite absorption coefficient. This is because at large energies the Airy states are plane wave like (with a small decay). The absorption coefficient reflects this by not decaying off but oscillates instead. Below 0.1 eV , the transitions are mostly to the decaying part of the Airy function.

6.5 Conclusion

By studying optical transitions between both bands and a band and the continuum, it has been discovered that these two transitions result in manifestly different forms for the absorption coefficient. Therefore, by experimentally studying this type of situation, the experimentalist should be able to differentiate between these transitions.

This has important consequences for ascertaining the electric field in a device. This is because the band to continuum transitions are more likely to occur at higher fields. Therefore if higher (or lower) fields, than one might expect, exist in the device, the absorption coefficient may then describe Stark-Airy instead of Stark-Stark (or Stark-Stark instead of Stark-Airy) type transitions.

Future work in this area could include an investigation of the effect disorder has on optical transitions in a superlattice. The wavefunction of the disordered superlattice could be calculated numerically using the transfer matrix technique and then substituted into Eq.(6.12) to obtain the absorption coefficient

7 ELECTRIC FIELD DEPENDENT LOCALISATION IN A SUPERLATTICE -AN ANALYTICAL TREATMENT

7.1 Introduction

The growth techniques that are used to form superlattices are very accurate and have resulted from the most up to date technology. However, techniques like MBE are still not perfect and this means, therefore, that the interfaces separating the different layers are not totally well defined. Indeed, even in the best devices, this interface can fluctuate by as much as a monolayer. This has also been shown to be the case in numerical simulations of MBE by Ghaisas and Madhukar (1985) and by Clarke and Vvedensky (1987) where fluctuations of one or two monolayers in the growth front are found. There has, however, been some progress in this area to improve the growth with Madhukar et al (1985) demonstrating experimentally and Clarke and Vvedensky (1987) showing via their numerical work that interruption of the growth process can allow the surface to relax resulting in smoother interfaces. However, this can then allow impurities that may be present in the growth chamber to deposit onto the surface which can result in further roughening.

The disorder which is induced by these fluctuations in the barrier and well widths can effect the extended Bloch like states found in the minibands resulting in the localisation of electrons and consequently a deterioration in the current that can flow. It is therefore important to

investigate this effect further, especially when there is a large electric field present.

Therefore, this and the next chapter will concentrate on the localising properties of a disordered superlattice in the presence of a large applied electric field. In this chapter a recursive transfer matrix method will be formulated and by using suitable approximations an analytical form for the amount of localisation an electron experiences in an electric field will be derived.

A chain of square barrier potentials with random heights will be used to model the superlattice. Furthermore, a chain of delta function potentials will also be used. Although these do not model a superlattice as well as the square barriers, they are interesting from a point of view of knowing how important the type of potential used is. In fact it will be shown that in an electric field the potential type can determine the resultant behaviour of the wavefunction as it propagates through the system. It will be assumed that the system is only one dimensional.

7.2 The Recursive Transfer Matrix Method

The transfer matrix method is an extremely common technique and has been used widely by many workers studying localisation (i.e. Pendry 1982 and Azbel 1980). However, there has not been much analytical work carried out on systems in the presence of an applied electric field. This is because an electric field parallel to the direction along which the transfer matrix acts greatly complicates any solution, especially analytical, to the problem. The complication is caused by a position dependent term in each transfer matrix related to the electric field. Therefore even after averaging over any disorder the transfer matrices remain distinct from one another and do not commute.

In the transfer matrix method the superlattice under

investigation is embedded in an infinite, perfectly ordered system. The wavefunctions for a single electron in the ordered regions are written

$$\begin{aligned}\Psi_0 &= e^{ik_0 x} + r e^{-ik_0 x} & -\infty < x < 1 \\ \Psi_N &= t e^{ik_N x} & x > N\end{aligned}\tag{7.1}$$

so that the disordered region extends from $x=1$ to $x=N$. The plane waves on either side of the superlattice are connected using the transfer matrix M to give

$$\begin{bmatrix} t \\ 0 \end{bmatrix} = M \begin{bmatrix} 1 \\ r \end{bmatrix}\tag{7.2}$$

r and t are the reflection and transmission amplitudes respectively and M is the transfer matrix for the whole superlattice and can be written

$$M = \prod_{i=1}^N m_i\tag{7.3}$$

m_i is the transfer matrix for a single barrier and is position dependent when there is an electric field present. The transmission coefficient T for an electron impinging on the superlattice is given by

$$T = \frac{k_N}{k_0} |t|^2\tag{7.4}$$

where k_N and k_0 is the electron's final and initial momentum respectively. T can be rewritten as

$$T = \frac{k_0}{k_N K_N^{11}}\tag{7.5}$$

where K_N^{11} is the one-one element of $\hat{K}_N$ and $\hat{K}_N = |M|^2$. Note that $|M|^2$ is the direct product $M M^*$ where M^* is the hermitian conjugate of M .

$\hat{K}_N$ can be written as

$$\hat{K}_N = |m(N)|^2 \hat{K}_{N-1} \quad (7.6)$$

The main advantage of using the transfer matrix approach when analysing disordered systems is illustrated clearly by Eq.(7.6). When the configurational average of $\hat{K}_N$ is taken, each transfer matrix can be averaged separately to give

$$\langle \hat{K}_N \rangle = \langle |m(N)|^2 \rangle \langle \hat{K}_{N-1} \rangle \quad (7.7)$$

Eq.(7.7) can now be used to evaluate the average 'resistance' such that

$$\langle T^{-1} \rangle = \frac{k_N}{k_0} \langle K_N^{11} \rangle \quad (7.8)$$

It should be noted here that the transmission coefficient is usually related to the resistance via the Landauer formula (Landauer 1970). However when a finite electric field is present the Landauer formula is no longer valid. There is a discussion of this point in the paper by Cota et al (1985).

In the papers by Anderson et al (1980) and Abrikosov (1981) it is argued that the logarithmic average is the statistically well behaved quantity and is therefore more relevant for experiment. This point has been discussed again in great detail by Stone et al (1981) and is somewhat controversial. In this paper the logarithmic average in addition to the arithmetic mean will therefore also be considered.

It can clearly be seen from Eq.(7.6) that averaging the logarithm of $\hat{K}_N$, as opposed to just averaging $\hat{K}_N$ as in Eq.(7.7), does not simplify the problem at all and that there is no simple way of relating the two averages except by a moment expansion (see Castello et al 1987). However, in the presence of an electric field and in the asymptotic limit, the evaluation of the logarithmic average is

straightforward and indeed turns out to be identical to the arithmetic mean. Before demonstrating this further the arithmetic mean will be considered.

In Eq.(7.8) only the first element of $\langle \hat{K}_N \rangle$ (which is a 4 x 4 matrix) is required to find the transmission coefficient, so the following recursion relation is derived

$$\langle K_N^{11} \rangle = \left[a(n) + \frac{b(n)}{S(n-1)} + \frac{c(n)}{S(n-1)S(n-2)} + \frac{d(n)}{S(n-1)S(n-2)S(n-3)} \right] \langle K_{N-1}^{11} \rangle \quad (7.9)$$

where

$$S(N-1) = \frac{\langle K_{N-1}^{11} \rangle}{\langle K_{N-2}^{11} \rangle} \text{ etc.} \quad (7.10)$$

and the coefficients $a(n), b(n), c(n)$ and $d(n)$ are simple combinations of elements of the matrices $\langle |m(N)|^2 \rangle$, $\langle |m(N-1)|^2 \rangle$, $\langle |m(N-2)|^2 \rangle$ and $\langle |m(N-3)|^2 \rangle$. For example, if $|m(N)|^2$ is a 2x2 matrix of the form

$$\begin{vmatrix} m_{11}(n) & m_{12}(n) \\ m_{21}(n) & m_{22}(n) \end{vmatrix} \quad (7.11)$$

the coefficients have the following form

$$a(n) = m_{11}(n) + \frac{m_{12}(n)m_{22}(n-1)}{m_{12}(n-1)} \quad (7.12)$$

$$b(n) = m_{12}(n)m_{21}(n-1) - \frac{m_{12}(n)m_{22}(n-1)m_{11}(n-1)}{m_{12}(n-1)}$$

Note that $c(n)$ and $d(n)$ do not exist for a 2x2 matrix.

Iterating (7.9) and writing it as an exponential gives

$$\langle K_N^{11} \rangle = \exp \left[\sum_{n=1}^N \ln \left[a(n) + \frac{b(n)}{S(n-1)} + \frac{c(n)}{S(n-1)S(n-2)} + \frac{d(n)}{S(n-1)S(n-2)S(n-3)} \right] \right] \quad (7.13)$$

For large N (large system size) the sum can be approximated by an integral and the S functions and the coefficients can be expanded as a Taylor series.

$$\text{i.e. } S(n-1) = S(n) - dS(n)/dn \dots$$

$$a(n-1) = a(n) - da(n)/dn \dots \quad (7.14)$$

etc

To zeroth order $dS(n)/dn$, $da(n)/dn$ etc and higher order derivatives can be neglected so that the coefficients $a(n)$, $b(n)$, $c(n)$ and $d(n)$ are now equivalent to the coefficients of the eigenvalue equation of $\langle |m(n)|^2 \rangle$. Namely

$$-\lambda^4 + a(n)\lambda^3 + b(n)\lambda^2 + c(n)\lambda + d(n) = 0 \quad (7.15)$$

where λ is the eigenvalue of $\langle |m(n)|^2 \rangle$. The validity and extension of this approximation is discussed in detail in the next section. To zeroth order

$$\langle K_N^{11} \rangle = \exp \left[\int_0^N \ln \lambda(n) dn \right] \quad (7.16)$$

Therefore to find the transmission coefficient, only the eigenvalues of the transfer matrix have to be integrated.

Consider now the logarithmic average of Eq. (7.6). As only the first element of $\hat{K}_N$ is required, the logarithm is

written

$$\ln(K_N^{11}) = \ln \left[\sum_{\mu} |m_{1\mu}(N)|^2 K_{N-1}^{\mu 1} \right] \quad (7.17)$$

Now if in the presence of an electric field, the ratios

$$\frac{|m_{1\mu}(N)|^2 K_{N-1}^{\mu 1}}{|m_{11}(N)|^2 K_{N-1}^{11}} \quad (7.18)$$

for $\mu \neq 1$ vanish in the $N \rightarrow \infty$ limit, then the following simple relation in the large N limit can be obtained

$$\langle \ln K_N^{11} \rangle \approx \langle \ln |m^{11}(N)|^2 \rangle + \langle \ln K_{N-1}^{11} \rangle \quad (7.19)$$

The elements of both the transfer matrices representing the chain of square barrier potentials and the chain of delta-functions do indeed satisfy the condition given by Eq.(7.18). Therefore Eq.(7.19) can be used to find the average of the logarithm so that a comparison can be made with the arithmetic mean obtained from (7.16).

7.3 Analysis of the Recursion Relation

In order to obtain some rigorous mathematical criteria as to the validity of the zeroth order approximation (7.16) and ways of going beyond it when necessary, consider the 2×2 example matrix (7.11). The generalisation to higher dimensional matrices is straightforward. From Eq.(7.9)

$$S(n) = a(n) + \frac{b(n)}{S(n-1)} \quad (7.20)$$

where $a(n)$ and $b(n)$ are given by (7.12). Using (7.20) the

following pair of equations can be derived

$$S^2(n-1) - S(n-1) \left[a(n-1) + \Delta(n-1) \right] - a(n-1)\Delta(n-1) + b(n-1) = 0 \quad (7.21)$$

$$\Delta(n) = a(n) - a(n-1) + \frac{[b(n) - b(n-1)]S(n-1) - b(n)\Delta(n-1)}{a(n-1)[S(n-1) - \Delta(n-1)] + b(n-1)} \quad (7.22)$$

$$\text{where } \Delta(n) = [S(n) - S(n-1)] \quad (7.23)$$

By writing

$$\Delta(n) = \Delta(n-1) + \delta(n-1) \quad (7.24)$$

it can be observed that zeroth order implies the neglect of $\Delta(n-1)$ in (7.21). This is equivalent to saying that in the solution of this quadratic

$$2S(n) = a(n) + \Delta(n) + \left[\{a(n) - \Delta(n)\}^2 + 4b(n) \right]^{\frac{1}{2}} \quad (7.25)$$

the following condition has been satisfied

$$\Delta(n) \ll a(n) \quad (7.26)$$

A condition that must be satisfied by the transfer matrix being used for sufficiently large n . Both transfer matrices that are used in this chapter do indeed satisfy this condition.

Systematic improvements to the zeroth order result are now quite straightforward. By treating the n 's as a continuous variable it is found that

$$\Delta(n) \sim \frac{dS(n)}{dn} \quad (7.27)$$

$$\delta(n) \sim \frac{d^2 S(n)}{dn^2} \quad (7.28)$$

Keeping $\Delta(n)$ to all orders is equivalent to substituting (7.22) into (7.21) with $\delta(n) \approx 0$. Thus the

effects to order $dS(n)/dn$ can be kept self-consistently by solving the pair of coupled quadratic equations (7.21) and (7.22). This procedure can now be extended to any desired accuracy by a single iteration. Note the interesting point that the zeroth order approximation leads to a pair, the first order to four and the second order to eight solutions etc. which is in complete analogy to a non-linear system. In the present case only the largest eigenvalue $\lambda_{\max}(n)$ needs to be considered since

$$T^{-1}(n) \sim e^{\sum_{n,\mu} \ln[f_{\mu} \lambda_{\mu}(n)]} \quad (7.29)$$

where f_{μ} is the coefficient for the μ th eigenvalue.

Most situations of interest, however, can indeed be solved analytically by using the pair of equations (7.21) and (7.22).

7.4 The Chain of Square Potential Barriers

The technique outlined above will now be used to evaluate the transmission coefficient for a chain of square potential barriers of random height in the presence of an electric field.

$$V(x) = \begin{cases} -eFx & (n+1)a-b/2 > x > na+b/2 \\ V_n - eFx & na+b/2 > x > na-b/2 \end{cases} \quad (7.30)$$

where V_n varies according to some probability distribution, e is the electronic charge and F is the electric field strength. This potential models the variation in the conduction band edge which results in the formation of a superlattice (see Fig. 1.1). In Cota et al (1985) the transmission coefficient was evaluated numerically for various length samples and analytically within the WKB approximation using this model. This reference used the ladder approximation and it will also be used here. It

greatly simplifies the form of the transfer matrix $m(n)$ while still maintaining sufficient accuracy (see Cota et al 1985 and Schwartz and Ting 1987). The full 'Airy function treatment' has been carried out for the regular superlattice numerically by Kelly (1987) and for the disordered superlattice by Schwartz and Ting (1987). $m(n)$ is now given by

$$m(n) = \begin{bmatrix} M_{11} & M_{12} \\ M_{12}^* & M_{11}^* \end{bmatrix} \quad (7.31)$$

where

$$M_{11} = \frac{k_1}{4k_3} (\alpha_{21}\alpha_{32}e^{ik_2b} + \alpha'_{21}\alpha'_{32}e^{-ik_2b})e^{i(k'_{13}na - k_{13}b/2)} \quad (7.32)$$

$$M_{12} = \frac{-k_1}{4k_3} (\alpha'_{21}\alpha_{32}e^{ik_2b} + \alpha_{21}\alpha'_{32}e^{-ik_2b})e^{-i(k_{13}na - k'_{13}b/2)}$$

and $\alpha_{21}=1+k_2/k_1$; $\alpha'_{21}=1-k_2/k_1$; $\alpha_{32}=1+k_3/k_2$; $\alpha'_{32}=1-k_3/k_2$

$$k_{13}=k_1+k_3 \ ; \ k'_{13}=k_1-k_3$$

$$k_1^2 = [E + F(na-b/2)]$$

$$k_2^2 = [E - V_n + F(na-b/2)] \quad (7.33)$$

$$k_3^2 = [E + F(na+b/2)]$$

E is the incident energy of the electrons and the k 's represent the momentum of the electrons in the barriers and wells.

The asymptotic form for the largest eigenvalue of the average of the direct product of (7.31) is

$$\lambda(n) = 1 - \frac{\langle V_n \rangle / 2}{Fna + E - Fb/2} + \left\langle \frac{V_n / 2 + Fb/2}{Fna + E - V_n - Fb/2} \right\rangle - \frac{Fb}{Fna + E + Fb/2} \\ + \text{terms of } 1/n^2 \text{ and higher}$$

$$\approx 1 - b/2na \quad (7.34)$$

$\ln \lambda(n)$ is now expanded for large n and only the first order terms are kept. To find the arithmetic mean this is substituted into equations (7.16) and (7.8) to give

$$\langle T^{-1}(N) \rangle_{N \rightarrow \infty} \sim N^{\frac{1}{2}} (1-b/a) \quad (7.35)$$

From Eq. (7.19) it follows that in the asymptotic limit, the logarithmic average also has this form, e.g.

$$\langle \ln T(N) \rangle_{N \rightarrow \infty} \sim \frac{1}{2} (b/a - 1) \ln N \quad (7.36)$$

These results show power law localisation of the electron which is in stark contrast to the exponential localisation one would expect without the electric field. The disorder, however, is not contained in the above equations. It shall be shown later that it comes in at a higher order. The effect of the potential is always present though and it does not matter how far above the barriers and wells the electron rises in energy. However if the width of the wells were equal to zero, so that the electrons were moving in a constant potential, b would have to be equal to a and T would become independent of the length of the system. This is exactly what one would expect.

In order to go beyond the strictly asymptotic limit and to recover the disorder, the Random Phase Approximation (RPA) (Thouless 1981) is used. RPA is valid for strong fluctuations in the height of the barriers which result in the cancelling out, on average, of multiple reflections. Consequently the 4×4 matrix $|m(n)|^2$ reduces to a 2×2 matrix of the following form

$$|m(n)|^2 \approx \begin{bmatrix} |M_{11}|^2 & |M_{12}|^2 \\ |M_{12}|^2 & |M_{11}|^2 \end{bmatrix} \quad (7.37)$$

Eq.(7.9) now has the form of Eq.(7.20), simplifying the calculations significantly. The eigenvalue of the average of this matrix is given by

$$\lambda_{\text{RPA}}(n) = 1 - \frac{\langle V_n \rangle / 4 + Fb/2}{Fn + E + Fb/2} + \left\langle \frac{V_n/4}{Fn + E - V_n - Fb/2} \right\rangle + \langle \cos(2k_2 b) \left[\frac{V_n/4}{Fn + E + Fb/2} - \frac{V_n/4}{Fn + E - V_n - Fb/2} \right] \rangle \quad (7.38)$$

In order to obtain the large N behaviour within the RPA, $\ln \lambda_{\text{RPA}}(n)$ is again expanded for large n and only the first order terms are kept. After integrating over the length of the system it is clear that the cosine term is negligible compared to the other two terms. However the fact that it exists is interesting and illustrates that there is weak oscillatory behaviour in the system with periodicity $(1/F) \{Fb/2 + \langle V_n \rangle - E + \pi^2/b^2\}$. The remaining terms give the following form for the average of the inverse of the transmission coefficient

$$\langle T^{-1}(N) \rangle_{\text{RPA}} \sim (Fn + E + Fb/2)^{\frac{1}{2}} (1 - b/a) \times \exp \left[\left[\frac{\langle W^2 \rangle / 4}{aF^2} \right] \times \left[\frac{1}{\varepsilon} - \frac{1}{N} \right] \right] \quad (7.39)$$

Where $\langle W^2 \rangle$ is the variance of the disorder and ε is the length scale below which the approximations are no longer valid. ε turns out to be of the order of E/F . Again, by using Eq.(7.19) to obtain the logarithmic average, it is found to be the same as Eq.(7.39). The power law term is still present above but is now dominated by the exponential term which contains the disorder parameter. This result agrees with the one obtained by Cota et al (1985) using the WKB approximation. However they kept only the exponential WKB contribution and neglected the prefactor contribution

to $\langle T^{-1}(N) \rangle$. Their result is recovered exactly if the $Fb/2$ term and the cosine term in (7.38) is dropped. In the limit that the exponential term tends to a constant (large system size) the neglected power law term dominates as illustrated in equations (7.35) and (7.36).

7.5 The Chain of Delta-Function Potentials

To gain further insight into the possible differences between the types of potential used to calculate the transfer matrix and also for completeness (as it is used by other workers) a chain of delta-function potentials in the presence of an electric field was also studied. In this case $V_n = b_n \delta(na)$ where b_n is the disorder parameter and is therefore analogous to V_n for the square barriers. The revised matrix elements of $m(n)$ become

$$M_{11} = \frac{1}{2k_2} (k_1 + k_2 + ib_n) e^{i(k_1 - k_2)na} \quad (7.40)$$

$$M_{12} = \frac{-1}{2k_2} (k_1 - k_2 - ib_n) e^{-i(k_1 + k_2)na}$$

where $k_1^2 = E + Fna$ and $k_2^2 = E + F(n+1)a$.

Again by using the Random Phase Approximation, the following form for the eigenvalue of the averaged transfer matrix is obtained

$$\lambda_{RPA}(n) = 1 + \frac{\langle b_n^2 \rangle / 2 - Fa/2}{E + Fna + Fa} \quad (7.41)$$

The asymptotic limit for λ is also of this form. Note that unlike the square barrier potentials there is no oscillatory behaviour in Eq.(7.41). $\ln \lambda_{RPA}(n)$ is expanded as before and only the first order terms are kept. After integrating over the length of the system and substituting this result into equations (7.16) and (7.8), the following expression for the average of the transmission coefficient

was obtained

$$\langle T^{-1}(N) \rangle_{N \rightarrow \infty} \sim \left[N \langle W^2 \rangle / 2aF \right] \quad (7.42)$$

As before this result is identical to the logarithmic average obtained using Eq.(7.19). The transmission coefficient is now completely power law localised with the exponent dependent on the amount of disorder and the strength of the electric field. Therefore even in the asymptotic limit the disorder plays a major role, totally unlike that for the square barrier potentials. This is caused by the delta-function potentials having an infinite height. Therefore no matter how much energy the electron gains from the field, it still cannot rise above the potential profile. This result agrees with those obtained analytically by Cota et al (1985) using the WKB approximation and by Castello et al (1987) using the transfer matrix approach.

7.6 Conclusion

The emphasis of this chapter has been the obtaining of tractable analytical results using lowest order approximations for the transmission coefficient as a function of system length. Even so, there has been excellent agreement with the results obtained by other workers using different techniques. Moreover, higher order results could easily be obtained using the method in this chapter simply by iterating Eq.(7.13) numerically if shorter, more practical structures are being investigated. In fact, in the next chapter this will be undertaken so that the transmission coefficient can be studied in much more detail, especially at the shorter length scales.

Finally it should be mentioned that although the work in this chapter has only been concerned with perfect coherence of the electron's wavefunction, the transfer

matrix technique can, if required, incorporate inelastic phase breaking collisions. This has been discussed by Band and Avishai (1986) and will not be included in the work contained in this thesis.

8 ELECTRIC FIELD DEPENDENT LOCALISATION IN A SUPERLATTICE -A NUMERICAL TREATMENT

8.1 Introduction

Now that approximate analytical results have been obtained for the transmission of an electron through a disordered superlattice, a much more detailed study will now be undertaken to investigate how an electron moves through a finite length superlattice in a large applied electric field. By treating this problem numerically it is possible to follow the electron step by step as it travels the length of the system. Furthermore, the approximations made in the last chapter can be checked. This is especially important for the RPA.

Hopefully the work carried out here will really show the true effect of the disorder induced by the variations in the layer widths. This is very interesting in the light of the previous analytical work which showed that in the asymptotic limit, the disorder did not effect the transmission coefficient. The question here is "How much will the disorder effect the transmission coefficient for shorter systems?".

8.2 The Numerical Recursive Transfer Matrix Method

In the analytical work in the previous chapter T^{-1} had to be averaged. Although it was also possible to obtain a form for $\langle \ln T \rangle$ in the asymptotic limit. However, in a

numerical calculation it is $\langle \ln T \rangle$ that has to be averaged. This comes from the fact that $M = \prod_1^N m_i$. This product can become very large and therefore can cause problems with the machine accuracy. Therefore to keep the numbers within certain limits the product is converted into a sum by taking $\ln M$. Moreover, there is a simplification here. $\ln T$ can be written

$$\ln T = \ln(k_N/k_0) - \ln M_{11} - \ln M_{11}^* \quad (8.1)$$

Because M_{11} is now required instead of $|M_{11}|^2$, only a 2×2 matrix needs to be solved, therefore the recursion relation is of the form

$$M_{11}^N = \left[a(n) + \frac{b(n)}{S(n-1)} \right] M_{11}^{N-1} \quad (8.2)$$

instead of the 4×4 recursion relation of Eq.(7.9). The averaging can now be simply carried out by repeating the calculation for a large number of systems. So now

$$\langle \ln T \rangle = \ln(k_N/k_0) - \langle \ln M_{11}^N + \ln M_{11}^{N*} \rangle \quad (8.3)$$

8.3 The Chain of Square Potential Barriers

The same chain of square potential barriers that were used in the last chapter are again used here to model the superlattice. To simulate the type of disorder induced by MBE, the widths of the barriers will be randomly varied, but the period of the lattice will be kept constant. Although the heights of the barriers were varied in the analytical work, varying their widths would have produced the same results. A square probability distribution ranging from $+D$ to $-D$ will be used for the disorder with D characterising the amount of disorder. The electric field will again be included using the ladder approximation.

Therefore the matrix elements are still given by (7.32)

8.4 Transmission Through a System of Varying Length

To find the form for the transmission coefficient as the length of the system is varied, Eq.(8.2) was numerically iterated for three amounts of disorder and at various electric fields for a system that ranged between 24 barriers and 50 barriers long. To produce two bands the height of the barriers was set at 0.4eV, the widths of the barriers set at 2.5nm and the period at 10nm. The incoming energy of the electron was set at about 0.06eV which puts it approximately in the centre of the lower band. The electric field was varied between zero and 0.05 in renormalised dimensionless units. A field of 0.05 would correspond to about $2 \times 10^6 \text{ Vm}^{-1}$. This means that at the greatest field and at the end of the sample the electron has gained enough kinetic energy to give it a total energy that is three times the height of the barrier.

The zero disorder case was studied first as a kind of reference to compare later results with. Fig. 8.1 displays the results for this case. Each graph in this figure displays data for a few fields. Graph(a) contains the curves for the lowest fields while graph(c) contains the highest fields. To understand how the electron is affected as it moves through the system in an electric field, each curve must be studied on the graphs, following through from one field to the next. Graph(a) shows $\ln(T)$ for the zero field case. As expected, the zero field curve is hardly changed as the length is increased. Increasing the field results in a linear decrease in $\ln(T)$ corresponding to an exponential decrease in T . The last curve on graph(a), $F=0.008$, and the first curve on graph(b), $F=0.01$, show that this decrease comes to an end resulting in the formation of a plateau. But further increases in the field results in another decrease in $\ln(T)$. This can be seen clearly at $F=0.02$. The final curves in graph(c) show that this

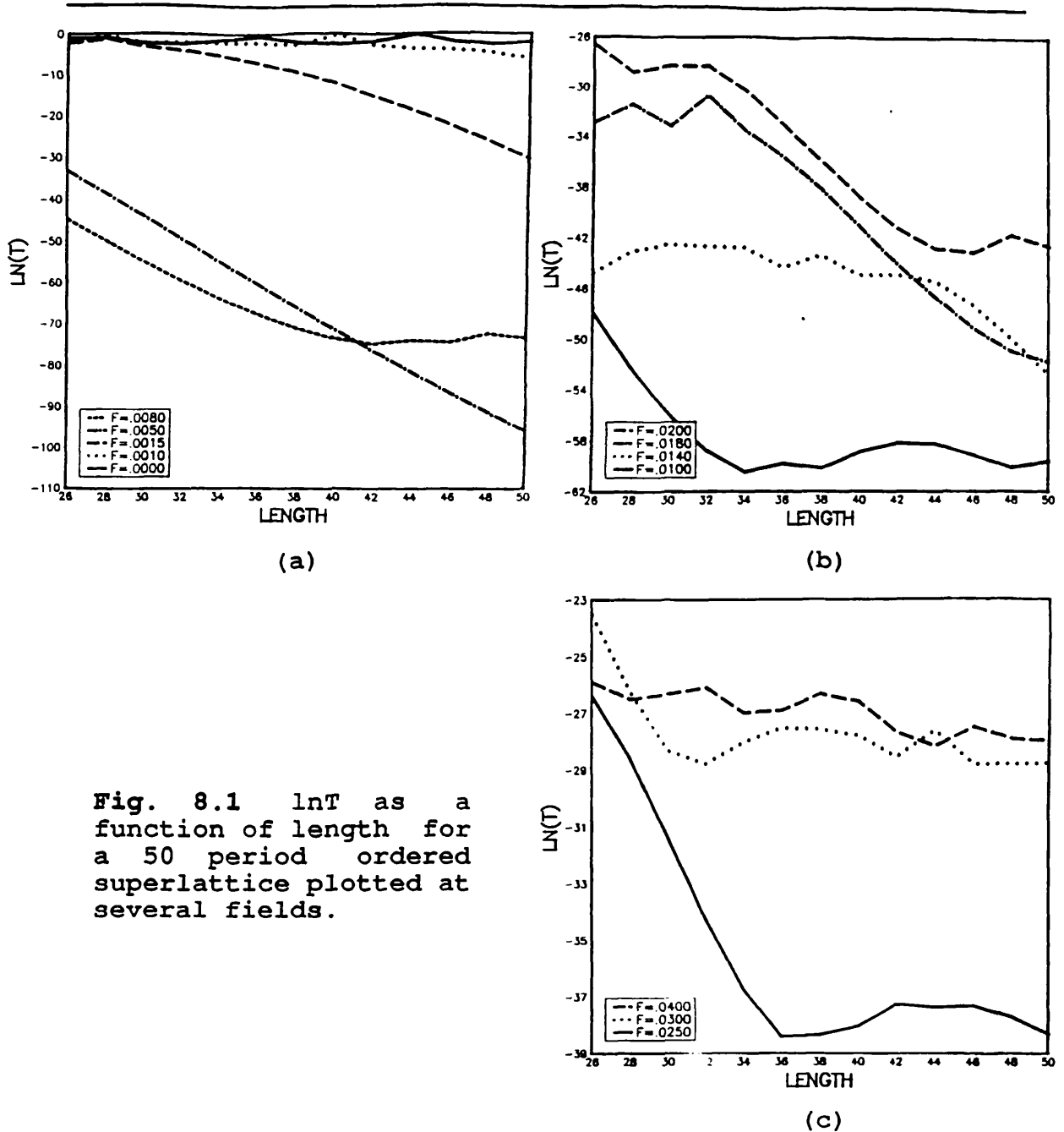


Fig. 8.1 $\ln T$ as a function of length for a 50 period ordered superlattice plotted at several fields.

decrease, like the previous one, again ends in a plateau.

To understand the origin of these plateaus and the exponential decreases, the kinetic energy the electron had gained from the applied field at the beginning and at the end of the slopes was calculated. The start of the first slope in graph(a) coincides with the electron having gained enough energy to leave the first band. The slope therefore occurs when the electron is Zener tunnelling from one band

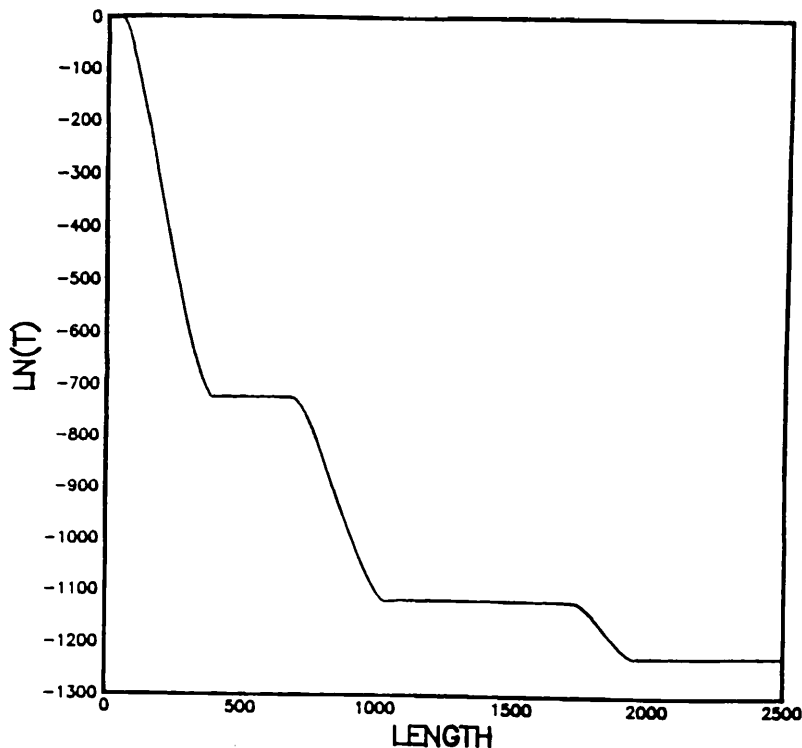
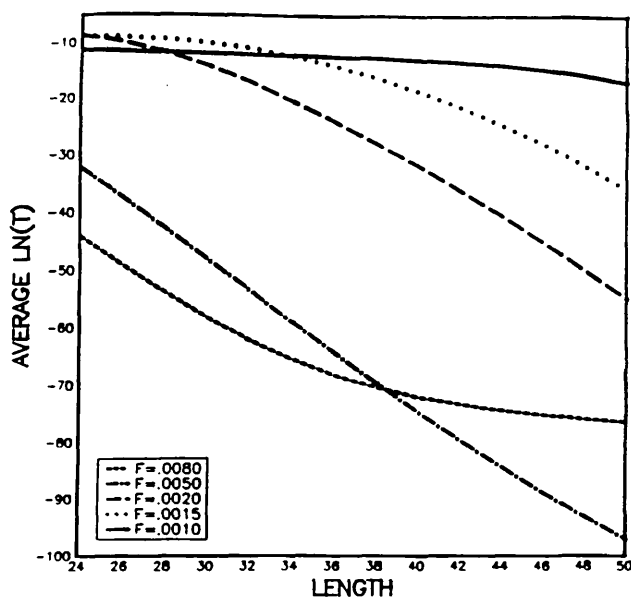


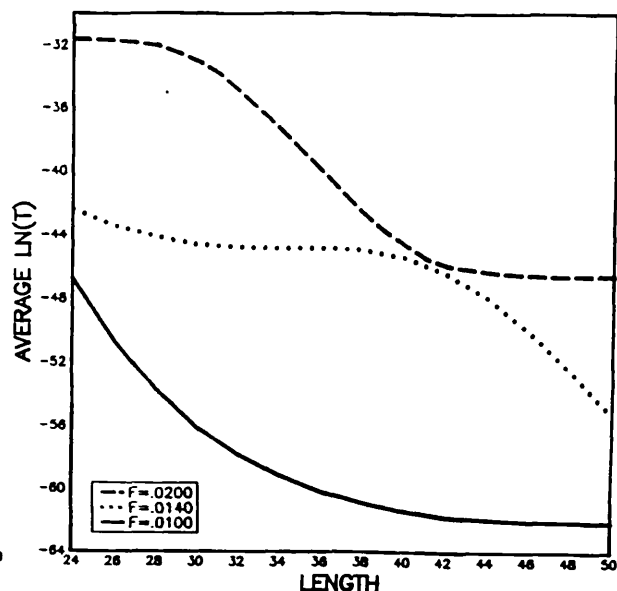
Fig. 8.2 $\ln T$ as a function of length for a 2500 period ordered superlattice at a field of $F=0.008$. Notice the sharp plateaus separated by regions of exponential localisation.

to the next. The end of this tunnelling period coincides with the electron entering the second band. It therefore can be concluded that the exponential decrease in the transmission coefficient results from the electron traversing the energy gap between the bands. When the electron is moving through a band the logarithm of the transmission coefficient remains constant.

To illustrate this point further, $\ln T$ against length was plotted for a system that was 2500 unit cells long in an electric field of 0.008 (Fig. 8.2). The plateaus and the slopes are clearly visible and their positions exactly coincide with the edges of the bands. The last decrease in $\ln T$ actually occurs above the barriers which means that there is a band gap located there. This point shall be returned to later.

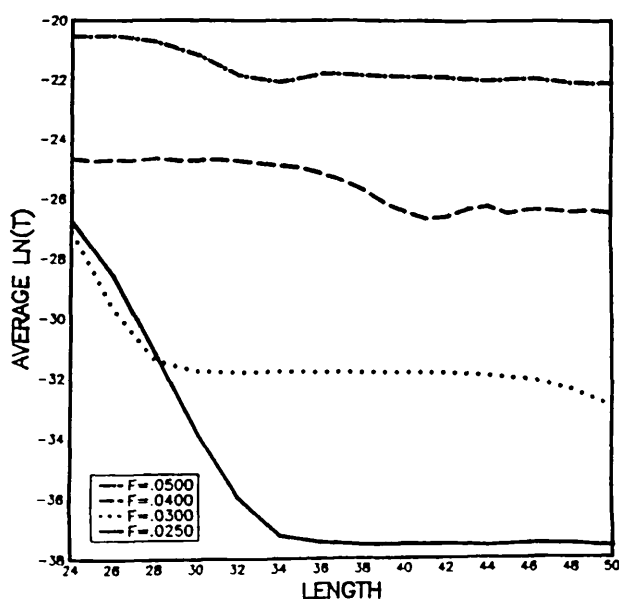


(a)



(b)

Fig. 8.3 The arithmetic average of $\ln T$ as a function of length for a 50 period weakly disordered superlattice plotted at several fields.



(c)

The effect disorder has on the results obtained for the ordered case will now be considered. The widths of the barriers were randomly varied by up to 10% ($D=2.5\text{\AA}$) of their original width. However, the period was kept constant so as not to effect the length of the system. As a way of discovering the effect a specific amount of disorder has on the system, the localisation length, given by the reciprocal of the gradient of a $\ln T$ v.s. length plot

at zero field, was measured. In the absence of an electric field the localisation is exponential and characterised by a localisation length which turns out to be 37 periods long for 10% disorder. This is therefore considered to be the weak disorder case.

The analysis that was carried out in the zero disorder case is repeated. Fig. 8.3 displays the three graphs showing the results at different fields. The same features that were visible in Fig. 8.1 for the zero disorder case clearly still exist. Namely the plateaus resulting from the electron moving through the bands and the exponential decrease in T characterising tunnelling through the gap. At the very low fields ($F \sim 0.001$) the transmission coefficient is not unexpectedly smaller for the disordered case than it was for the ordered one. However, as the field is increased further, there becomes little difference between the transmission coefficient of either the ordered or the disordered superlattice.

Now consider the stronger disorder regime. In this case the widths of the barriers were varied by up to 50% ($D=1.25\text{nm}$). Experimentally this would correspond to a very poorly grown MBE sample or a sample consisting of very narrow barriers. From a $\ln T$ v.s. length plot for the zero field case the localisation length was measured to be ~ 1.4 periods which confirms that this is the strong disorder case. However, as the field is increased it can be seen from Fig. 8.4 that the same plateaus and the same slopes that were present in Fig. 8.1 and Fig. 8.3 are again present here and that their positions with regard to the energy gained by the electron from the field is also the same. It should be noted that an extra decrease in $\ln T$ is visible in graph(c) of both Figs. 8.3 and 8.4 (it is more pronounced in 8.4). It occurs when the energy of the electron is above the wells and is caused by a small energy gap that exist there. This is the same gap that can be clearly seen in Fig. 8.2. Again the absolute values for the transmission coefficient are hardly effected by the disorder.

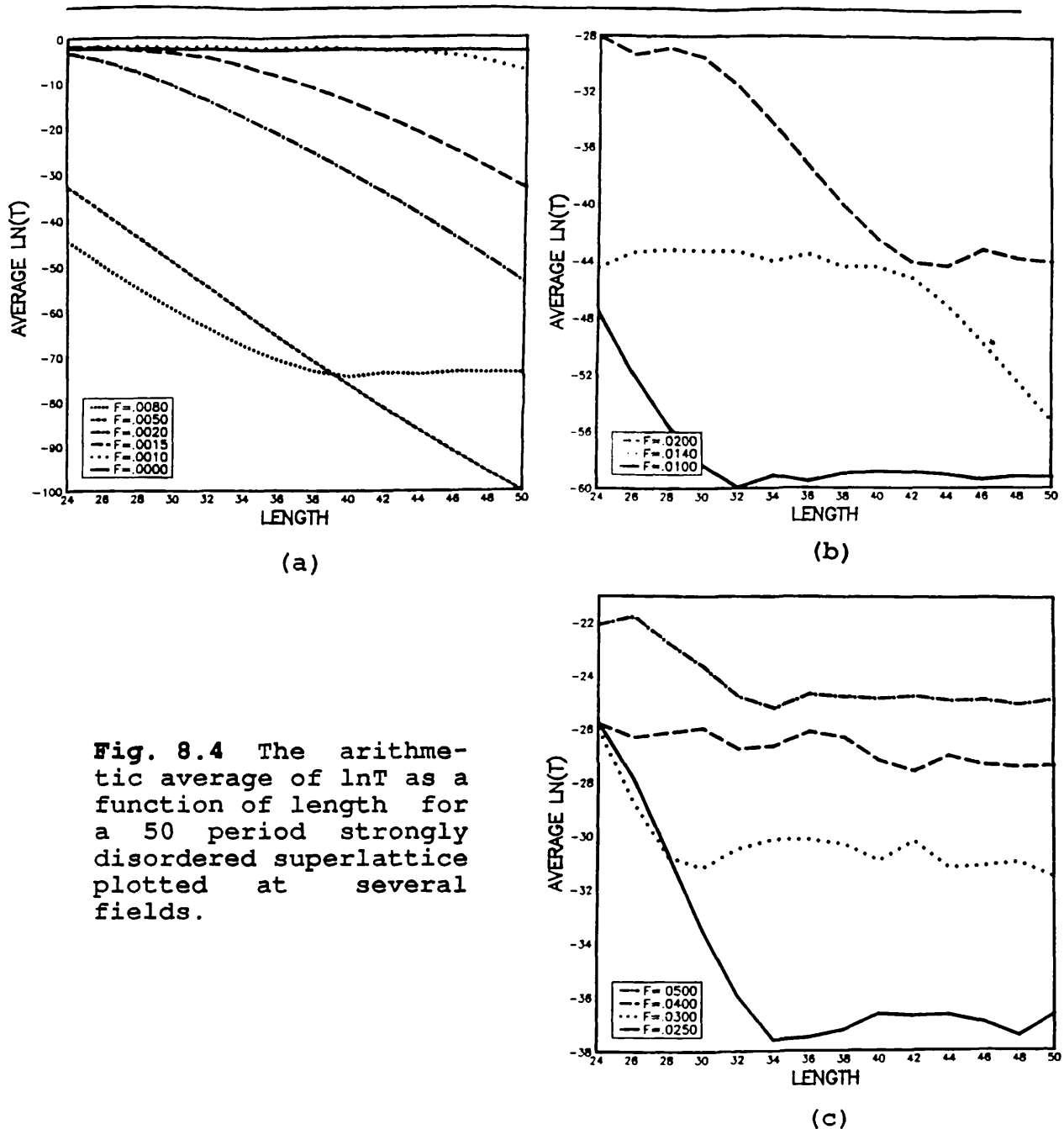


Fig. 8.4 The arithmetic average of $\ln T$ as a function of length for a 50 period strongly disordered superlattice plotted at several fields.

It can, therefore, be concluded that the form for $\ln T$ as the length is varied is only very weakly dependent on the disorder in the presence of an applied electric field. The fact that the positions of the plateaus visible in $\ln T$ are in the same place regardless of the amount of disorder is very interesting but not totally surprising. The disorder that was introduced does not entirely destroy the band structure, but instead reduces the transmissivity of

the states within the band and also produces some new states around the edge of it. Namely, all the states within the band become localised with a localisation length that depends upon the amount of disorder. In three dimensions a mobility edge may exist in the band, separating localised states from extended states. When an electric field is applied such that the Stark length becomes less than the length of the system, whether the states are either localised or extended becomes unimportant because the bands are now sloping. This effectively localises all the states, even in an ordered system. Consequently, the important quantity here is the density of states which by showing where energy states exist, give the starting and ending points of the plateaus and slopes in $\ln T$. For an averaged system, the width of the density of states is hardly effected by the disorder. Therefore, the positions of the plateaus and slopes, in turn, remain unchanged.

Now consider the RPA. In the analytical work carried out in the previous chapter this approximation was used to produce results much more simply. This was because $|M_{11}|^2$ could be obtained from a 2×2 matrix instead of a 4×4 matrix. The RPA produces no similar simplification in the numerical calculation as a 2×2 matrix is already being considered. However, it is still used so that a comparison can be made with the exact results.

Fig. 8.5 displays the results at different fields. The first thing to notice is the localisation length, obtained from the zero field curve, is less than 0.34 periods even though a disorder in the barrier of only 50% was used. Therefore disorder has a much stronger effect when used within the RPA. This is because multiple reflection that can increase the transmission of the propagating wave are neglected. This also means that no bands are produced and so the plateaus in $\ln T$ are not expected to be observed. Nevertheless, from Fig. 8.5 it can be clearly seen that the overall form for $\ln T$, especially in the asymptotic limit, is similar to that

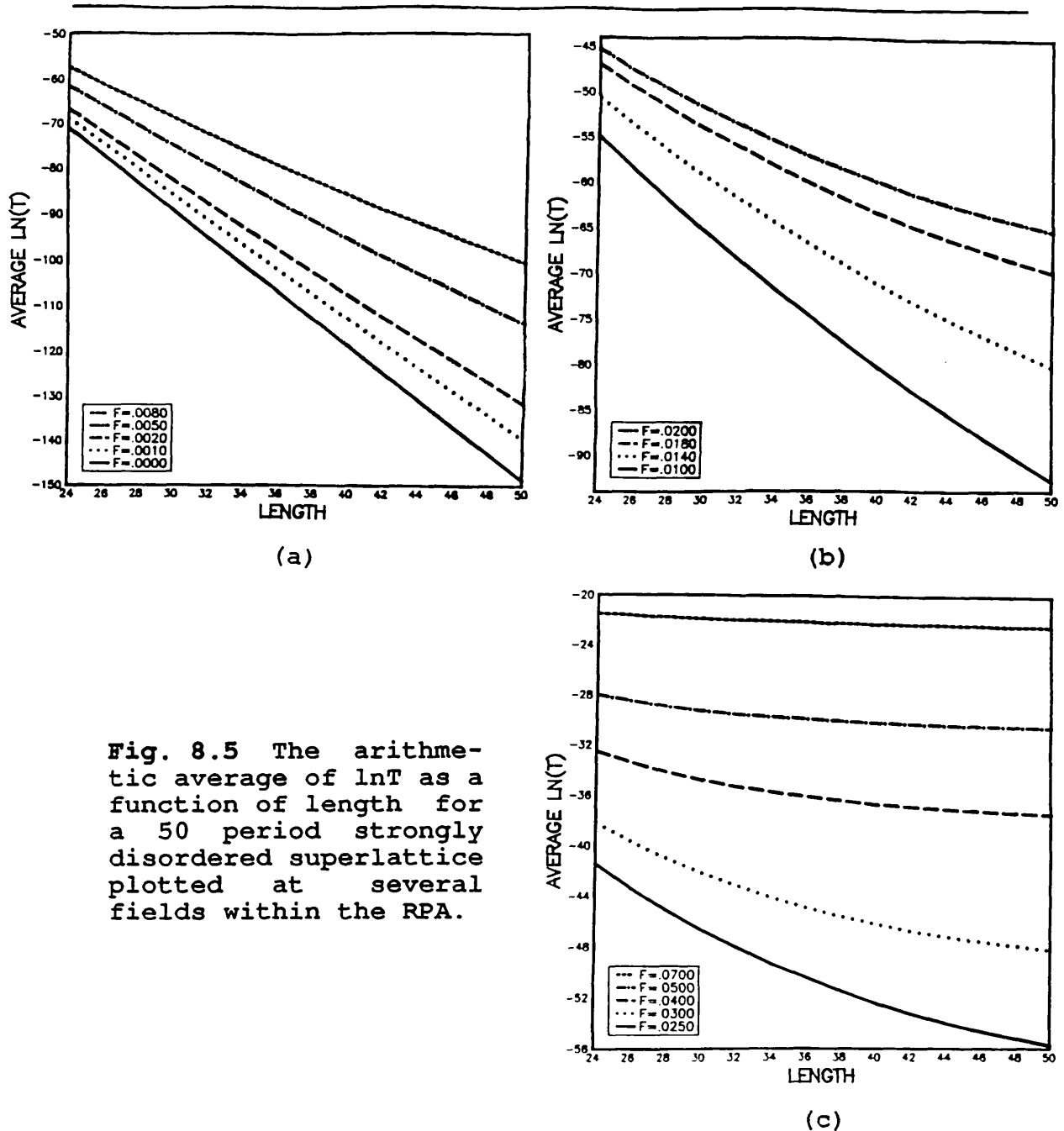


Fig. 8.5 The arithmetic average of $\ln T$ as a function of length for a 50 period strongly disordered superlattice plotted at several fields within the RPA.

given in Figs. 8.1, 8.3 and 8.4. Therefore although RPA enhances the effect of disorder and does not reproduce the features resulting from the bands, it can still be used to obtain general forms or trends which are especially applicable in the asymptotic limit.

In similar studies made by Cota et al (1985) and Schwartz and Ting (1987) of $\ln T$ against length in a disordered one dimensional chain of square barriers, they

found jumps in $\ln T$. In the paper by Cota et al they attributed this to one of two possible causes, Zener tunnelling or the energy of the electron matching a special 'delocalisation' point in the spectrum. By studying their data one finds that the jumps always occur when the electron has gained a particular amount of kinetic energy. On the other hand, Schwartz and Ting believe their jumps are caused by tuning the electron's energy to the energy of a localised state. The jumps are exactly analogous to the slopes evident in Figs. 8.1, 8.3 and 8.4. They are caused by the electron Zener tunnelling through the band gap and therefore always occur at the same electron energy. The jumps in Cota et al's data are probably caused by the energy gap that is present far above the tops of the barriers (eg the last slope in Fig. 8.2).

8.5 The Transmission Coefficient as a Function Field

A question that may be more pertinent to experiment when the V-I characteristics of a device are under consideration, is the effect varying the field has on the transmission coefficient. First consider the idealised case of a perfectly ordered superlattice. It has already been mentioned that the application of an electric field results in the formation of a Stark ladder in each band. These ladders of energy states move apart when the field is increased and it was shown in chapter 5 that at specific values of the field, ladders belonging to different bands come into resonance. The same kind of effect can be expected if the field is varied while the incoming energy of the electron is kept constant. Indeed Fig. 8.6 shows that as the field is varied, resonances occur in $\ln T$. The incoming energy of the electron is set to be in the gap between the two bands so that the effects due to only one band are observed.

The distance between the resonances increases which points to the possibility that they could be caused by the

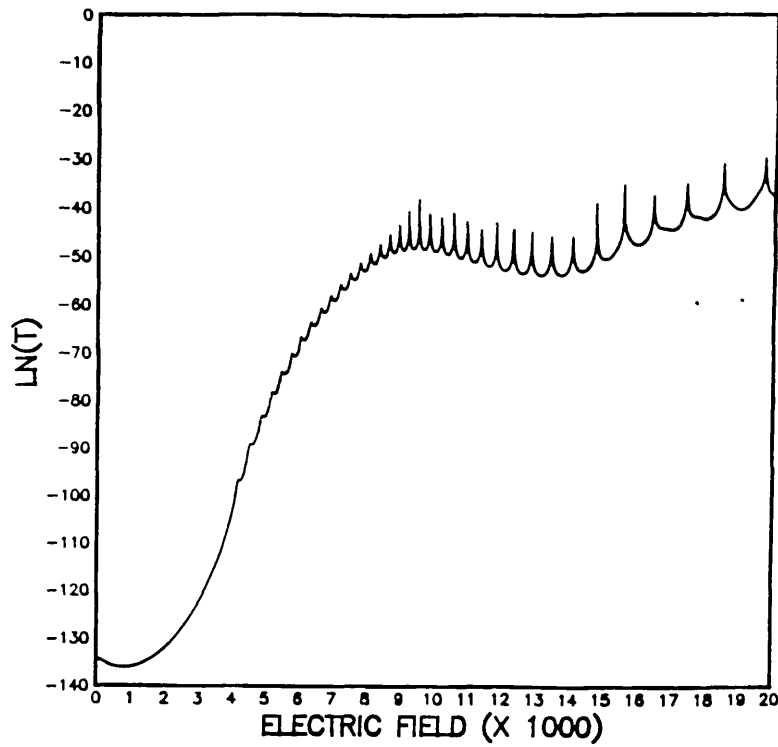


Fig. 8.6 $\ln T$ versus electric field for a ordered superlattice. Only tunnelling through one band is being considered.

states in the Stark ladders. This is because the position of the levels in a Stark ladder are given by (Saitoh 1972)

$$E_n = eF_n a + E_0 \quad (8.4)$$

where n is the Stark label and E_0 is the energy origin of the ladder. Therefore, resonance between the Stark levels and the initial energy E_i occurs when the field is given by

$$F_r = \frac{E_i - E_0}{nea} \quad (8.5)$$

For all the resonances given in Fig. 8.6, F_r against $1/n$ was plotted (Fig. 8.7). Apart from the first section of the graph, the points lie on a very good straight line.

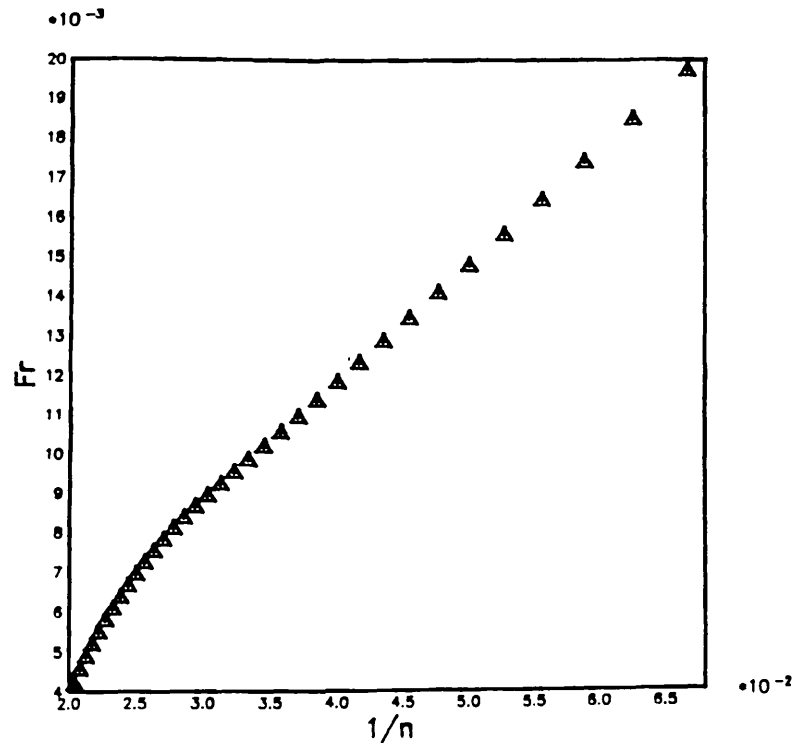


Fig. 8.7 A plot of the field at which the resonances in Fig. 8.6 occur versus the reciprocal of the indices characterising the Stark states.

The deviation from the straight line at low fields is caused by boundary conditions. At the edges of the sample the distance between Stark levels is not eFa but is much larger. This coupled with the fact that the resonances at low fields are caused by the electron using these edge states as paths of conductance results in the curve in Fig. 8.7. These resonances, therefore, are similar to the Zener resonances observed in chapter 5. However, these resonances are caused by a coupling of the Stark states to states that exist outside the sample.

The above calculations were repeated with the initial energy of the electron below both bands. In Fig. 8.8 the consequences of having to traverse both Stark ladders can now be observed with two sets of resonances present and superimposed upon each other. The resonances resulting

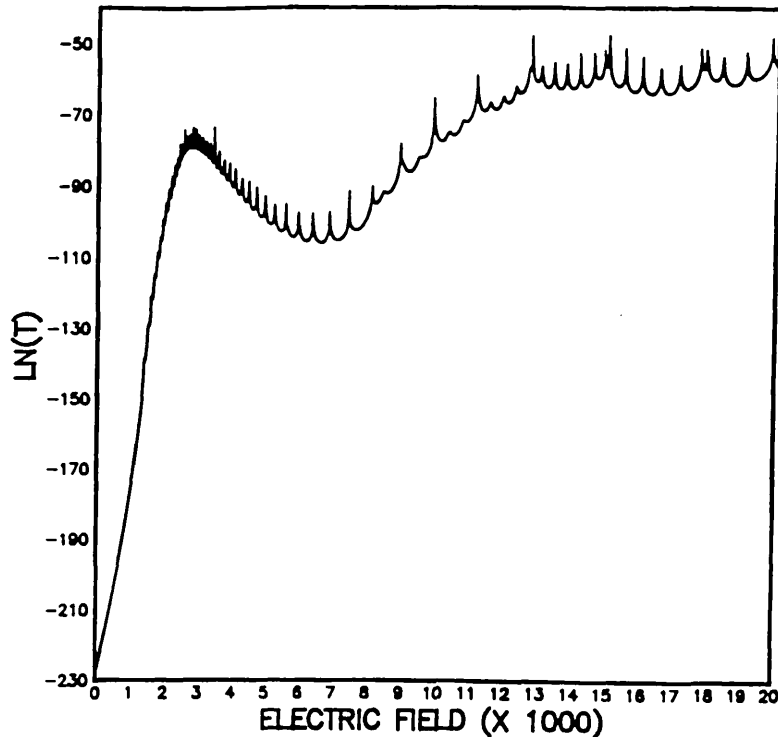


Fig. 8.8 $\ln T$ versus electric field for a ordered superlattice. Tunnelling through two bands is now being considered.

from the Stark ladder in the higher band start at a much higher field (~ 0.008) and are initially visible as much weaker resonances.

The introduction of disorder into the system must clearly affect the Stark resonances. To understand how, consider the derivation of a Stark ladder in an ordered system given in chapter 4. Schrödinger's equation for a periodic system in the presence of an electric field was

$$\left[\frac{p^2}{2m^*} + V(x) - eFx \right] \Psi(x) = E \Psi(x) \quad (8.6)$$

By translating this equation by a lattice constant it was shown that a Stark ladder could be produced (see Eqs.(4.1),

(4.2) and (4.3)). However, with disorder in the system $V(x+a)$ no longer equals $V(x)$. Therefore, translating (8.6) by a lattice constant now gives

$$\left[\frac{p^2}{2m^*} + V(x) + V'(x) - eFx \right] \Psi(x+a) = (E+eFa) \Psi(x+a) \quad (8.7)$$

where V' is the extra potential caused by the disorder and can be written

$$V'(x) \Psi(x+a) = \varepsilon \Psi(x+a) \quad (8.8)$$

Therefore a random energy ε is added on to the Stark energy $E+eFa$. Nonetheless, the important result is that the Stark ladder still exists, albeit somewhat modified, even in the presence of disorder.

To confirm this $\ln T$ against field was plotted for two samples, one with strong disorder (50%) and one with weak disorder (10%). The electron was injected between the two bands so that the effect of just one Stark ladder is again observed. No averaging was carried out on these samples so that the numerical results obtained would give an indication of the type of output that might be observed experimentally when every sample is unique and not an average.

Fig. 8.9 shows that the results in the weak disorder limit are not very different from the results in the ordered case given by Fig. 8.6. It can be observed though that the positions of the resonances are not well defined and are actually slightly random. The amount by which the positions of the resonances can fluctuate is related to the disorder D . Consequently, as expected the positions of the resonances in the strong disorder case (Fig. 8.10) are even more random. If these results were averaged to simulate thermal or similar effects, then of course these rather elegant resonances would not exist.

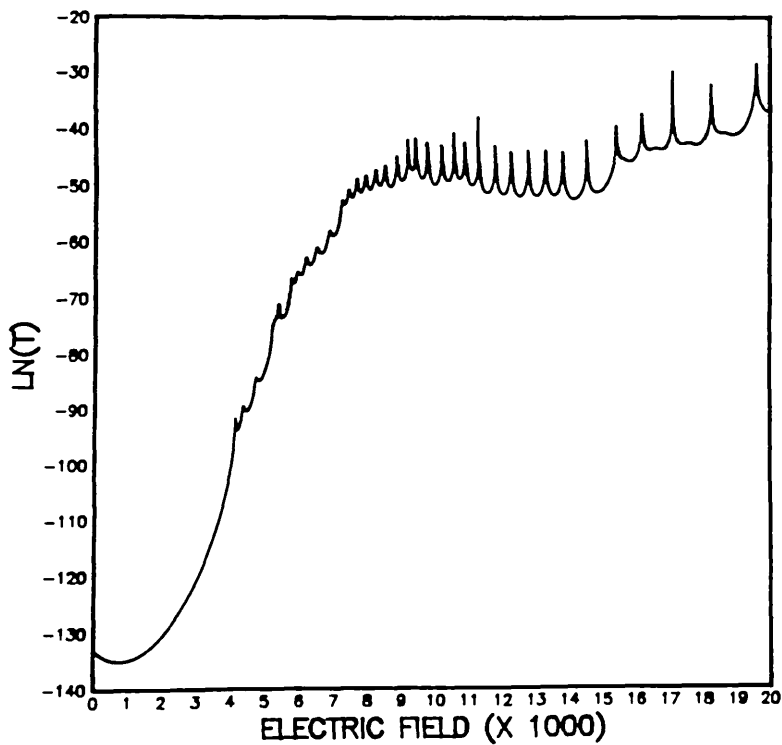


Fig. 8.9 $\ln T$ versus electric field for a weakly disordered superlattice.

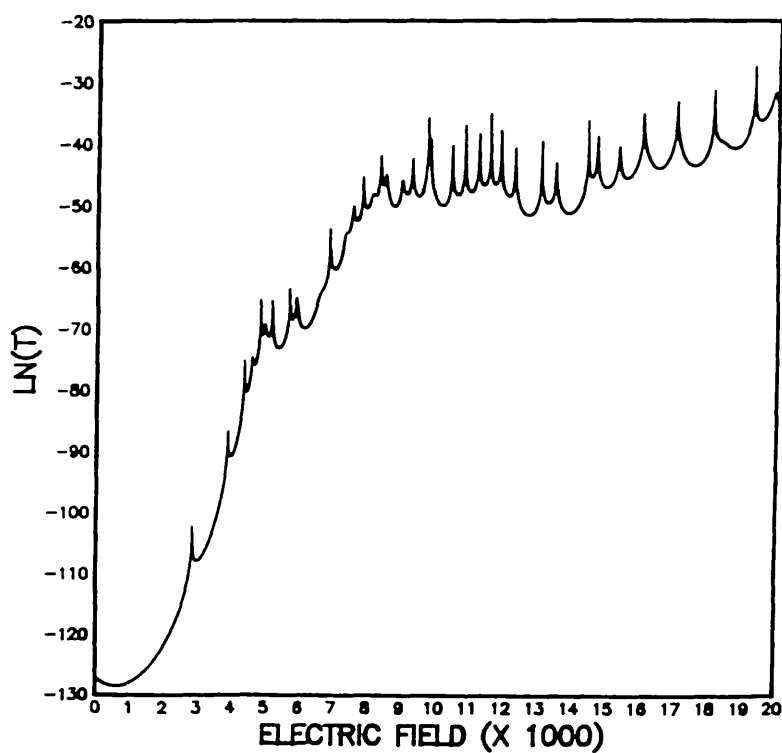


Fig. 8.10 $\ln T$ versus electric field for a strongly disordered superlattice.

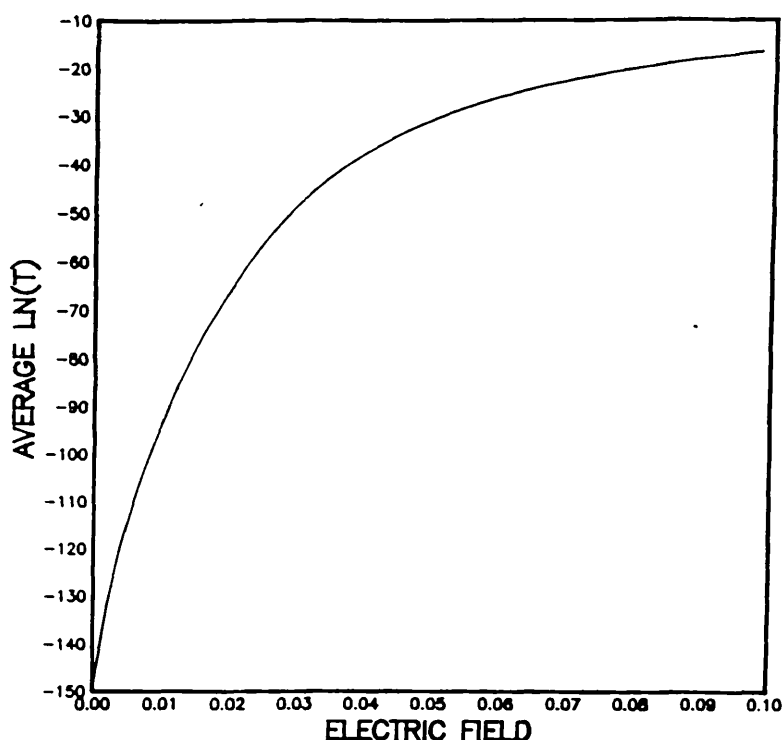


Fig. 8.11 The arithmetic average of $\ln T$ plotted against field for a disordered superlattice within the RPA.

$\ln T$ was also studied within the RPA (Fig. 8.11). Application of the field results in a very rapid initial rise in $\ln T$ which seems to be exponential in T . However, as the field is increased further $\ln T$ starts to tail off, tending to a constant value in the asymptotic limit. Again by comparing Fig. 8.11 with Fig. 8.6, it can be seen that RPA reproduces the course features of the results and probably simulates the effect of averaging the data given in Figs. 8.9 and 8.10.

8.6 Conclusion

The present work now shows that the amount of disorder present in a superlattice in an electric field is not

important if the electric field is such that the Stark length is less than the system size. What effects the transport properties much more is the number of bands and their widths. This is because $\ln T$ has two functional dependences on position depending on whether the electron's energy (this includes the energy it has gained from the field) puts it in one of the bands or one of the gaps when it has reached the end of the system.

Although it has been shown that disorder does not seem to effect the overall amplitude of the transmission much, it can effect certain features like the position of the resonances caused by the Stark states. However, the main point is that disorder does not destroy the Stark ladder, it just modifies it into a ladder whose rungs are randomly varied around specific positions. The possibility therefore exists of using the Stark resonances that might occur in the current as an indicator of the amount of disorder in a particular sample.

9 MAGNETOTRANSPORT IN MQW STRUCTURES

9.1 Introduction

So far, this thesis has been concerned with transport in MQW and superlattice structures under the influence of an electric field only. In this chapter the effect of applying a magnetic field perpendicular to the electric field (i.e. parallel to the layers) will be considered. This type of configuration has not been studied to any appreciable degree or extent. Much work has instead been channelled into the situation where the magnetic field is perpendicular to the 2DEG of the wells. This has provided some very interesting physics (i.e. Klitzing et al 1980).

The effect a magnetic field has on a GaAs/AlGaAs superlattice structure has been studied experimentally by Davies et al (1987). Their superlattice, however, was not uniform but consisted of two superlattices coupled via a thick barrier. Consequently most of the bias was dropped across this one barrier misaligning the superlattice minibands on either side. Apart from this effect, the bands themselves were fairly unaffected by the electric field (i.e. they did not slope).

The V-I characteristics of this structure at zero magnetic field were found to contain a region of NDR resulting from this misaligning of the minibands. The application of the magnetic field perpendicular to the electric field was observed to have two effects on the NDR. At low magnetic fields it moved to higher biases, but as the magnetic field was increased to over 10T the NDR completely disappeared. Similar work has been carried out

by Eaves et al (1986), Hickmott (1987) and by Lebens et al (1988) who studied tunnelling through a single barrier system with crossed electric and magnetic fields. Johnson et al (1987 and 1988) have theoretically studied the more general problem of how a magnetic applied parallel to an interface effects the energy states across that interface.

In this chapter the effect of a weak magnetic field ($\leq 3T$) on the transport characteristics of a MQW structure will be investigated numerically using the transfer matrix technique of chapter 8.

9.2 The magnetic field parallel to the layers

Consider a MQW or superlattice structure where the well/barrier period is in the x direction, and the electrons are plane waves in the other two dimensions. The application of magnetic field B in the z direction results in the following Hamiltonian in the Landau gauge

$$H = \left[p_x^2 + p_z^2 + \left[p_y - eBx \right]^2 \right] \frac{1}{2m^*} - eFx + V(x) \quad (9.1)$$

The ansatz is now made that the solution to Schrödinger's equation with the above Hamiltonian has plane waves in the y and z directions, therefore

$$\left[\frac{p_x^2}{2m^*} - eFx + V(x) + \frac{e^2 B^2 x^2}{2m^*} - \frac{eB}{m^*} xp_y \right] \Psi_v(x) = E_v \Psi_v(x) \quad (9.2)$$

where v labels the Landau levels. Therefore the application of an electric field results in two extra terms in the Hamiltonian, a quadratic 'oscillator' term and a linear term. This linear term can be absorbed into the

electric field so that

$$eF' \rightarrow eF + \frac{eB}{m^*} p_y \quad (9.3)$$

If the approximation is now made that B is sufficiently weak such that the cyclotron radius a_0 where

$$a_0^2 = \frac{\hbar}{eB} \quad (9.4)$$

is much greater the width of the barrier which separates any two quantum wells, then the effect B has on the matrix elements between neighbouring wells can be neglected. Therefore, the only effect Eq.(9.2) has is to shift the energy of one well with respect to its neighbour by

$$-eFb + \frac{e^2 B^2}{2m^*} b^2 - \frac{eBb}{m^*} p_y \quad (9.5)$$

Note that now the energy an electron gains by crossing the barrier between two wells in the presence of a B field is no longer just a function of position but also a function of the electron's transverse momentum p_y . This can be viewed in the following way. Classically the magnetic field will cause electrons to perform cyclotron motion. Therefore after travelling a distance b in the x direction their velocity in the y direction will increase by an amount Beb/m^* . This can be represented as causing a lateral shift of the k_y dispersion relation. Now consider the situation if b is the width of a barrier. Although the electric field shifts the origin of the y and z dispersion relations so that there is a mismatch in energy, the lateral shift caused by the B field can then allow an electron with a specific k_y to cross the barrier (see Fig. 9.1). This can therefore suppress the NDR caused by the energy mismatch and it was this effect that Davis et al observed in their double section superlattice.

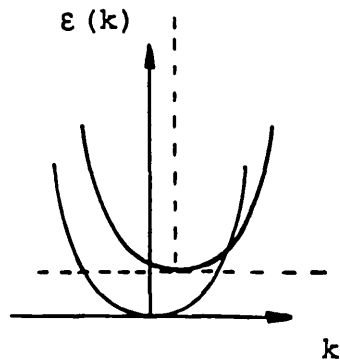


Fig. 9.1 A schematic diagram showing the 2DEG dispersion curves for two wells separated by a barrier in the presence of crossed electric and magnetic fields. The electric field causes a shift in energy between the two wells while the magnetic field results in a lateral displacement that can realign the energies at a particular momentum.

9.3 Crossed E and B Fields in a MQW Structure

The above formulation can now be incorporated into the transfer matrix method by simply modifying the k momenta in each well and barrier section given in Eq.(7.33) by the amount given in Eq.(9.5) above. The linear term now exaggerates the effect of the electric field term to further increase the kinetic energy of the electron as it moves through the system. However, there is also a positive quadratic term which reduces the energy of the electron. In the limit of a weak magnetic field the linear energy terms will dominate over a distance of several quantum wells. However, the quadratic positive term will eventually take over causing the localisation of the electron into a cyclotron orbit.

Two types of structures were investigated using this technique. Both were MQW structures (or superlattices) consisting of ten barrier/well periods, but the electric

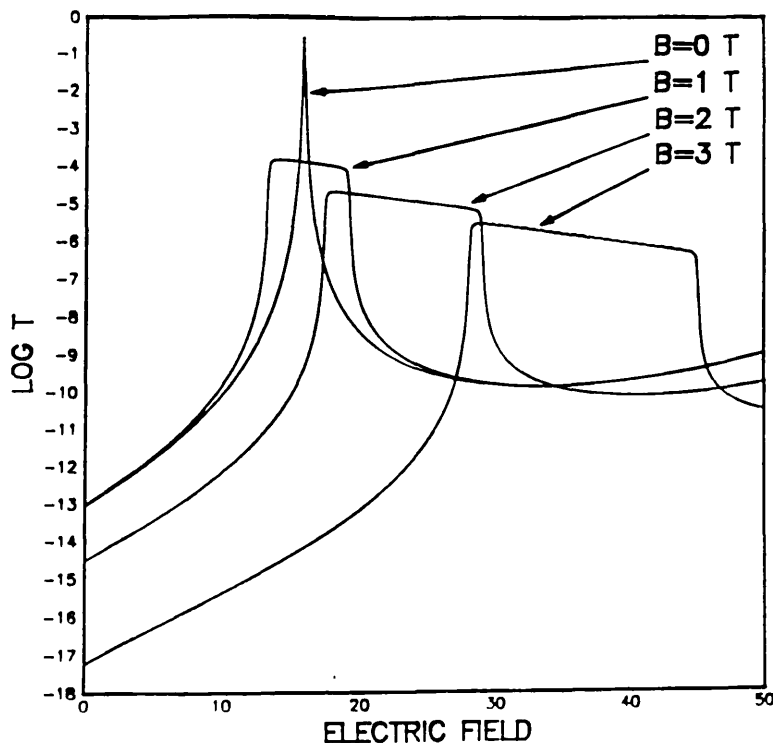


Fig. 9.2 $\ln T$ versus electric field for a 10 period superlattice with all the electric field dropped across the last barrier. The resonance is displayed for four magnetic fields.

field effected them both in different ways. In the first sample, all the field was dropped across the last barrier. This could therefore represent a double barrier structure or a system similar to Davis'. Fig. 9.2 shows the results obtained for four magnetic fields, 0, 1, 2 and 3 Tesla. The width of the barriers and wells were set to $25\text{\AA}$ and $75\text{\AA}$ respectively and $F=1$ corresponded to about $5 \times 10^3 \text{ V/cm}$. p_y was summed from zero to $1.5 \times 10^{-26} \text{ Kgms}^{-1}$.

At zero magnetic field the peak caused by the alignment of the bound state in the last well and the incident energy of the electron is clearly visible at $F=1.5$. As B is increased two effects are observed in complete agreement to that found by Davis. First the peak becomes much broader as the bound state becomes resonant with electrons at different p_y . This obviously strongly

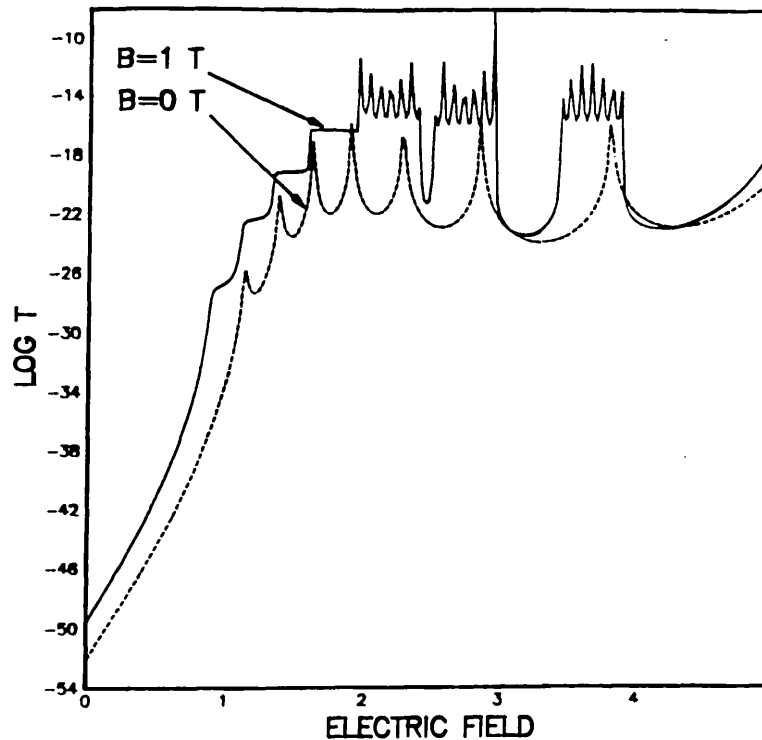


Fig. 9.3 $\ln T$ versus electric field for a 10 period superlattice with the electric field now dropped uniformly across the whole structure. The Zener resonances are shown for two values of the magnetic field.

effects the NDR. Then as the magnetic field is increased further up to 2T, the peak moves to higher biases and becomes even more broader as the bound state becomes resonant with even more electrons, all with different transverse momentum. Finally an increase of B to 3T was found to further exaggerate these features.

The plateau formed on the now broadened peak is caused by the sum over the transverse momentum p_y in the following way. An electron with a particular p_y will form a particular V-I curve. Studying an electron with a different p_y is equivalent to studying an electron with the previous p_y but at a different electric field (this can be seen from Eq.(9.3)). Therefore the electron with this new p_y produces the same shape V-I curve as the electron with the previous p_y but it is now shifted along the electric

field axis. Consequently, peaks in the V-I curves are formed into plateaus.

In the second structure the field was allowed to drop uniformly across the whole system. This would result in the formation of the now familiar Stark states and Stark ladder, although now because the system is so short, these states may be strongly effected by the boundaries. Fig. 9.3 shows the results obtained for zero magnetic field and for a field of 1T. At $B=0$ the same Stark resonances that were studied in chapter 8 are visible. The application of the magnetic field causes a broadening out of the resonances to such an extent that the ones at low biases almost disappear completely. However, the resonances at the higher biases turn into groups of seven mini-resonances. These exist because the magnetic field makes it possible for electrons with different p_y to tunnel resonantly via other Stark states. In a real system these resonances would be smeared out by scattering.

An effect observable in Fig. 9.3 and which is contrary to the features in Fig. 9.2 and the observations made by Davis is that the broadened NDR has moved to lower biases instead of higher biases, resulting in a negative magnetoresistance. This results from the fact that the linear terms in (9.5) are dominating over the quadratic term. In Fig. 9.2 the opposite was true.

9.4 Conclusion

Although the present technique for dealing with perpendicular magnetic fields is only very approximate, the initial results that have been obtained have reproduced the essential features observed experimentally. However, the limiting factor in these calculations has been the cyclotron radius which can become comparable to a barrier/well period at fields of 3T or less. Therefore to be able to study the effects of magnetic fields of 20T, so that comparisons can be made with experiment, this

technique has to be improved.

A first step to achieving this could come from a study of a tight-binding model in the presence of an electric and a magnetic field. For example, consider the effect a magnetic field has on the matrix element $t_{\perp}$ perpendicular to the layers and the matrix element $t_{//}$ parallel to the layers of a MQW or superlattice structure. Using the Landau gauge and incorporating the magnetic Peierls phase factor into the matrix elements allows the magnetic field to be included in the matrix elements as a phase factor in the following way

$$\begin{aligned} t(n, n+1; m) &\rightarrow t_{\perp} \text{ (i.e. unchanged)} \\ t(n, n-1; m) &\rightarrow t_{\perp} \end{aligned} \quad (9.6)$$

$$\begin{aligned} t(n; m, m+1) &\rightarrow t_{//} e^{-in\Phi a_y} \\ t(n; m, m-1) &\rightarrow t_{//} e^{in\Phi a_y} \end{aligned} \quad (9.7)$$

where a_y is the lattice constant in the y direction, n and m denote the position of the n'th and m'th site in the x and y directions respectively and $\Phi = eBd/\hbar$. Only nearest neighbour interactions are allowed. The z direction has been ignored as it is unaffected by the magnetic field. By again making the ansatz that the wavefunctions are plane wave like with momentum k_y in the y direction, the following effective one dimensional Hamiltonian is obtained

$$\begin{aligned} H = \sum_n \{ eFd n + 2t_{//} \cos[(k_y + n\Phi) a_y] \} c_n^{\dagger} c_n \\ + \sum_{n, n'} t_{\perp}(n, n') c_n^{\dagger} c_{n'}, \end{aligned} \quad (9.8)$$

The inclusion of the magnetic field has led to a shift in energy in each well given by $2t_{//} \cos(k_y + n\Phi) a_y$. Therefore for a given k_y , the energy change experienced by an electron as it tunnels between adjacent quantum wells in crossed electric and magnetic fields is given by

$$-eFd + 2t_{//} [\cos(k_y + \Phi) a_y - \cos(k_y a_y)] \quad (9.9)$$

Expanding the cosine for small arguments recovers the linear and quadratic terms given in Eq.(9.5) where the effective mass is now given by $\hbar^2/2t_{//}a_y^2$.

The solution of (9.8) numerically could lead to some very interesting results. This equation was studied by Hofstadter (1976) without the electric field and produced a very rich energy spectrum. However, to study very high magnetic fields, the matrix elements in (9.8) would have to be dependent on the size of the magnetic field.

CONCLUSION

This thesis has not been an attempt to study every aspect of transport, in every detail, in every type of MQW or superlattice structure. But by focusing in on what has been considered to be the important and salient features of perpendicular transport in these systems of reduced dimensionality, it is hoped that this thesis contains the foundations to allow, by simple extensions of the work, the investigation of transport in many more specific systems. It then becomes the job of a device engineer to find out how particular amounts of doping, or how novel constructions of superlattices might effect the movement of electrons.

There are two stages which must be overcome in theoretical work before any experimental predictions can be made. First, the model has to be selected which, hopefully, matches the real physical situation as closely as possible. For example, for the superlattice a chain of square well potentials were used. These may not represent the complete picture, but one hopes, and indeed expects, that the results that arise from this model can go some way to reproducing the experimental results. Then there is the method by which the results are obtained. This could be first order perturbation theory in the form of Fermi's Golden Rule, or the transfer matrix method were the incoming electrons are represented by plane waves of infinite extent.

These approximations could be superseded, of course, but not without a tremendous increase in the amount of work. This also goes for the models that were used. All

of these were chosen so as to give the most accurate results without making the work required totally impractical. And indeed, it is a testament to methods like the tight-binding approximation which produce results that so closely resemble experiment but which are tractable and simple to use. However, whether it will prove possible to observe things like the Zener resonances studied in chapter 5 remains an open question.

It is, therefore, hoped that this thesis has, by their use, illustrated the relative merits of these common theoretical techniques that are used in condensed matter physics. Furthermore, by using both analytical and numerical methods, the relative merits of these two ways of solving a problem can be scrutinised.

It is customary in a concluding chapter of a thesis to attempt to answer the question "what next?". Well first of all more work needs to be carried on the magnetic field problem. This has formed only a minor part of this thesis, and there is still plenty of work to be carried out.

Secondly there is the many particle aspect of transport. Nearly all the work in this thesis is performed within the single electron approximation which is a good approximation most of the time and reproduces experimental data very well. However, the fact that there could exist large numbers of electrons in the device, especially in highly doped systems, would lead to some very interesting and novel physics. For example, an inhomogeneity in a tunnelling device could hold up the movement of electrons resulting in a build up of charge. This will in turn alter the field across the inhomogeneity which will react back on the flow of electrons. Therefore the problem has to be treated self-consistently and time-dependently. This line of research could result in some very interesting and novel non-linear physics in the fields of noise and chaos.

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