

Single-particle relaxation times and scattering times in a 2D electron gas

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Abstract. We examine the effect of the different spatial widths of successive subbands on the calculation of the single-particle relaxation and scattering times when up to two subbands are occupied. It is shown that, firstly, the single-particle relaxation time for the second subband is always larger (by a factor of two or more) than that for the ground subband and, secondly, the scattering time for the second subband is sometimes larger and sometimes smaller than that for the ground subband (depending on the electron concentration in the second subband) in qualitative agreement with recent experimental data.

1. Introduction

When an electron in a momentum eigenstate is subjected to scattering mechanisms there are two time constants that are significant. The first is the single-particle relaxation time which is a measure of the lifetime of the state as a result of all possible transitions. It can be determined experimentally from the amplitude of the Shubnikov-de Haas oscillations (Fang *et al* 1988). The second time constant is the scattering time (or the transport time) which determines how fast the momentum is dissipated by those transitions that are effective in changing momentum. It can be obtained experimentally from the mobility μ through the relation

$$\mu = e\tau_s/m^* \quad (1)$$

where e and m^* are the magnitude of the electron charge and effective mass respectively.

There has been a great deal of discussion recently about the relationship between the scattering times τ_s and the single-particle relaxation times τ_r when two subbands are occupied in a modulation doped GaAs/GaAlAs heterojunction. Such occupation may occur at high temperatures or high concentrations of carriers. It leads to two important effects. Firstly the transport involves an intersubband scattering mechanism which decreases τ_s and τ_r for the first subband when the second begins to be occupied. Secondly the screening of the scattering potentials includes contributions from all the occupied subbands (Stern 1978).

Experimental data (Fang *et al* 1988, Van Houten *et al* 1988, Smith *et al* 1988, Smith and Fang 1988) indicated that τ_s for the second subband (τ_{s2}) is always larger than that for the first subband (τ_{s1}) and that the scattering time for the first subband τ_{r1} is sometimes larger and sometimes smaller than the corresponding quantity for the second subband τ_{r2} . This is in contradiction to previous theoretical calculations (Mori and Ando 1980)

and experimental results (Störmer *et al* 1982, Englert *et al* 1983) which indicate that τ_{12} is always smaller than τ_{11} . The observed difference of behaviour between the two times raises a number of problems. A possible answer to these problems lies in the larger spatial width of the second subband which in some cases is up to three times that of the first subband (Ando 1982). The increased width increases the second-subband scattering times considerably when the spacer layer is much smaller than the width of the first subband.

In this paper we calculate the effect on τ_s and τ_t of the occupation of the second subband using the multisubband transport theory of Siggia and Kwok (1970) and taking into account the difference of the spatial widths of the subband wavefunction.

2. Poisson's equation

Following the approach of Stern and Howard (1967) we use the two-dimensionally Fourier transformed Poisson equation for an ionised impurity of charge e at $z = z_0$ where the Cartesian coordinate z is measured perpendicular to the plane of the 2DEG. We write x and y for the Cartesian coordinates in the plane of the 2DEG and we assume that the permittivity is independent of x and y . Thus we obtain

$$\epsilon(z) \frac{d^2 A(q, z)}{dz^2} + \frac{d\epsilon(z)}{dz} \frac{dA(q, z)}{dz} - q^2 \epsilon(z) A = -2Ze\delta(z - z_0) - \rho_{\text{ind}}(q, z) \quad (2)$$

where $\epsilon(z)$ is the permittivity at the position z . In equation (2) $A(q, z)$ and ρ_{ind} are the two-dimensional Fourier transforms of the potential and the induced charge density. In a linear screening approximation and neglecting intersubband coupling (Stern 1978) we have

$$\rho_{\text{ind}}(q, z) = - \sum_i \beta_i(q) g_i(z) A_i(q) \quad (3)$$

where i labels the subbands and $\beta_i(q)$ and $g_i(z)$ are the dielectric function and the normalised charge density for this subband respectively. Finally

$$A_i(q) = \int_{-\infty}^{\infty} A(q, z) g_i(z) dz \quad (4)$$

By solving equation (2) and using equations (3) and (4) we obtain for A_i

$$A_i(q) = -2Ze \int_{-\infty}^{\infty} G(z, z') g_i(z) dz \quad (5)$$

$$+ \sum_{j=1}^n \beta_j(q) A_j(q) \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} G(z, z') g_i(z) g_j(z') dz dz'$$

where $G(z, z')$ is the Green function for equation (2). Assuming now that we have the same dielectric constant everywhere in our material so that $\epsilon(z) = \epsilon$, a constant, the Green function $G(z, z')$ is (Morse and Feshbach 1953)

$$G(z, z') = (-1/2\epsilon q) e^{-q|z-z'|} \quad (6)$$

3. General theory of the relaxation time and the scattering time

In the case of a 2DEG with two subbands occupied we approximate the subband wavefunctions from the following sinusoidal formulas:

$$\Psi_n = \sqrt{2/\alpha_n} \cos(n\pi z/\alpha_n) \quad 0 \leq z \leq \alpha_n \quad (7)$$

and

$$\Psi_n = 0 \quad z \leq 0 \quad z \geq \alpha_n \quad (8)$$

where $n = 1$ and 2 indicates the subband and α_n is the spatial width of the wavefunction for the n th subband which depends on n (Stern and Das Sarma 1984, Walukiewicz *et al* 1984, Ando 1976, Yokoyama and Hess 1986, Ando 1982). Mori and Ando (1980) use a self-consistent variational wavefunction in which the two widths are the same. Our elementary wavefunctions are not self-consistent but they are good enough to show the essential significance of the different spatial widths of the two subband wavefunctions for the phenomena under discussion.

When the system of coupled equations (5) is solved we find for A_i (Stern 1978)

$$A_i = 2Ze \frac{G_i + (G_i G_{jj} - G_j G_{ij})}{1 + \beta_j G_{jj} + \beta_i G_{ii} + \beta_i \beta_j (G_{ii} G_{jj} - G_{ij} G_{ji})} \quad (9)$$

where $i \neq j$, $i, j = 1, 2$ and

$$G_i = \int_0^{\alpha_i} G(z, z') g_i(z) dz \quad (10)$$

and

$$G_{ij} = \int_0^{\alpha_i} \int_0^{\alpha_j} G(z, z') g_i(z) g_j(z') dx dz'. \quad (11)$$

We use here (Ando *et al* 1982, Stern 1967) the RPA dielectric function. For the second subband, RPA yields the same results as the Thomas–Fermi approximation only when the density of electrons in subband 2, n_{s2} , is comparable with that in the first subband, n_{s1} . On the other hand, when n_{s2} is much smaller than n_{s1} the Fermi wavenumber in subband 2 becomes very small and the associated screening wavenumber is greatly reduced below the Thomas–Fermi value.

The intersubband matrix element is

$$\langle k_1 | V | k_2 \rangle = \int_0^{\alpha_1} A(q, z) \Psi_1 \Psi_2 dz = A_{12}(q). \quad (12)$$

When subband 2 is unoccupied the inverse of the single-particle relaxation time in subband 1 is obtained by integrating $P_1(k, k')$ over all k' :

$$\tau_{s1}^{-1} = \int P_1(k, k') dk'. \quad (13)$$

Here $P_1(k, k')$ is the scattering rate from a state $k = (k_x, k_y)$ to a state k' . This transition rate is given by Fermi's Golden Rule (Schiff 1967)

$$P_1(k, k') = (2\pi/\hbar) |\langle k | V(x, y) | k' \rangle|^2 \delta(E(k') - E(k)) \quad (14)$$

where $V(x, y)$ is the scattering potential integrated over all z with a weighting factor $g_1 =$

$\Psi_1\Psi_2$. We can see immediately that the matrix elements are the A_i we give in equation (9). It follows that (Stern and Howard 1967)

$$\tau_{s1}^{-1} = \Lambda \int_{z_0}^{\infty} \int_0^{2\pi} |A_1|^2 n(z') d\theta dz' \quad (15)$$

where θ is the scattering angle, $\Lambda = m^*e^22\pi/\hbar^3$ and $n(z')$ is the density of the impurities at a plane z' from the interface and z' is integrated from the spacer layer thickness $z_0 = 1.5$ nm to infinity. In our case $n(z')$ is a constant with value 10^{18} atoms cm^3 .

When the second subband is occupied another channel is opened to the electrons in subband 1 and τ_{s1} becomes

$$\tau_{s1}^{-1} = \Lambda \int_{z_0}^{\infty} \int_0^{2\pi} (|A_1|^2 + |A_2|^2)n(z') d\theta dz' \quad (16)$$

where i is the subband index and $ij = 1, 2, i \neq j$ and $n(z')$ is the density of the impurities at a plane z' from the interface and z_0 is again 1.5 nm.

Calculations of the scattering times are much more difficult. Stern (1978) calculates them on the assumption that intersubband scattering may be neglected. Consequently he does not find a decrease in the mobility in the first subband when the second subband begins to be occupied. The calculation has been improved by Mori and Ando (1980) who take account of intersubband scattering which is also included in our calculations.

Siggia and Kwok (1970) give the details for many subbands. Applying their general equation (88) for two populated subbands and solving the resulting equations we have

$$\tau_{ii} = (P_j + P_{ij})/(P_iP_j - P_{ij}P_{ji}) \quad (17)$$

where $i \neq j$,

$$P_i = \frac{2\pi}{h} \int_{z_0}^{\infty} \int |\langle k' | V(x, y) | k \rangle|^2 (1 - \cos \theta) \delta(E_i(k) - E_i(k')) n(z') dk' dz' \\ + \sum_{i \neq j} \frac{2\pi}{h} \int_{z_0}^{\infty} \int |\langle k' | V(x, y) | k \rangle|^2 \delta(E_j(k') - E_i(k)) n(z') dz' dk' \quad (18)$$

and

$$P_{ij} = \frac{2\pi k_j}{\hbar k_i} \int_{z_0}^{\infty} \int_0^{2\pi} |\langle k' | V_{ij} | k \rangle|^2 \cos \theta n(z') dz' d\theta. \quad (19)$$

In these equations V_{ij} is the scattering potential averaged over all z with a weighting factor $g_{ij}(z) = \Psi_i(z)\Psi_j(z)$.

4. Comparison with experiment

An interpretation of the early data on two-subband transport leads to the conclusion that the mobility of the electrons in the ground subband is larger than that for those in the first excited subband (Stern and Howard 1967). This is in agreement with the theoretical results of Mori and Ando. The main reason for this is that the Fermi wavevector in the first excited subband is much smaller than that of the ground subband.

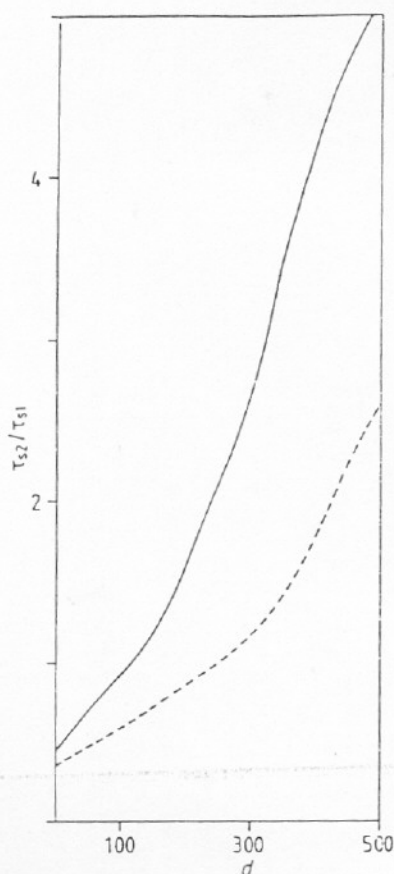


Figure 1. Plots of the ratio τ_{s2}/τ_{s1} against the difference between the subband widths in units of the Bohr radius $k_F a_0 = 0.0133$ (full curve) and 0.0123 (broken curve).

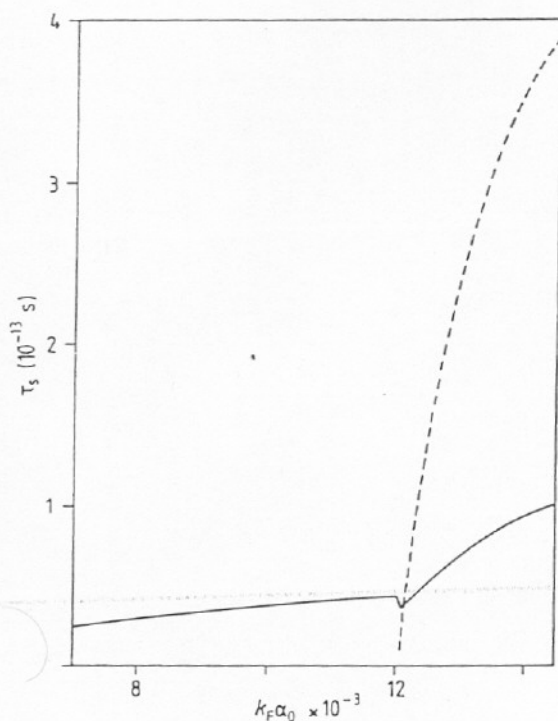


Figure 2. Plots of τ_{s1} (full curve) and τ_{s2} (broken curve) against $k_F a_0$ when $d = 450$ and $z_0 = 1.5$ nm.

However, recent experimental work shows a different behaviour. Fang *et al* (1988) measure τ_{t1} , τ_{t2} , τ_{s1} and τ_{s2} for a GaAs/GaAlAs heterojunction with a spacer layer thickness of 1.5 nm and find that $\tau_{s2} = 3.0 \tau_{s1}$ and the overall mobility increases by a factor of 1.5 after the occupation of the second subband. This suggests that $\mu_2 > \mu_1$ and $\tau_{t2} > \tau_{t1}$ (Fang *et al* 1988). Smith and Fang (1988) find $\mu_2 > \mu_1$ and $\tau_{s2} = 2.2 \tau_{s1}$. On the other hand Van Houten *et al* (1988) and Smith *et al* (1988) find $\tau_{t2} < \tau_{t1}$. Thus the experimental data indicate that τ_{s2} is always larger than τ_{s1} but τ_{t2} is sometimes larger and sometimes smaller than τ_{t1} .

At first sight these results are very perplexing because they indicate that there is no well defined relationship between τ_s and τ_t as has been supposed (Das Sarma and Stern 1985). We show below that the explanation lies in the variation of the spatial width of the subband wavefunctions which has been ignored by Mori and Ando (1980) because they were investigating a superlattice rather than a heterojunction.

In figure 1 we plot the ratio τ_{s2}/τ_{s1} at 0 K for $k_F a_0 = 0.0133$ (full curve) and 0.0123 (broken curve) against the normalised difference in the spatial subband widths $a = (\alpha_2 - \alpha_1)/a_0$ for a spacer layer thickness $z_0 = 1.5$ nm and a first subband width $\alpha_1 = 23$ nm. Here a_0 denotes the Bohr radius in free space. The values of z_0 and α_1 describe the samples used by Fang *et al* (1988). In particular, α_1 is the square well width corresponding to the subband occupancies which they quote. The values of k_F chosen illustrate what happens when the second subband begins to be occupied and when

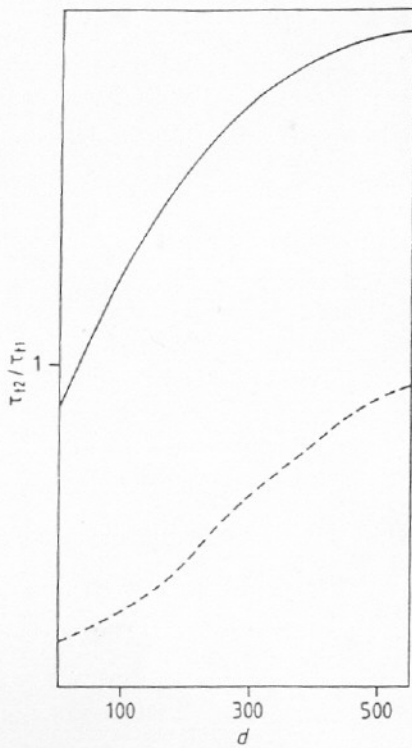


Figure 3. Plots of the ratio τ_{12}/τ_{11} against d for $k_F a_0 = 0.0133$ (full curve) and 0.0123 (broken curve) when $\alpha_1 = 23$ nm and $z_0 = 1.5$ nm.

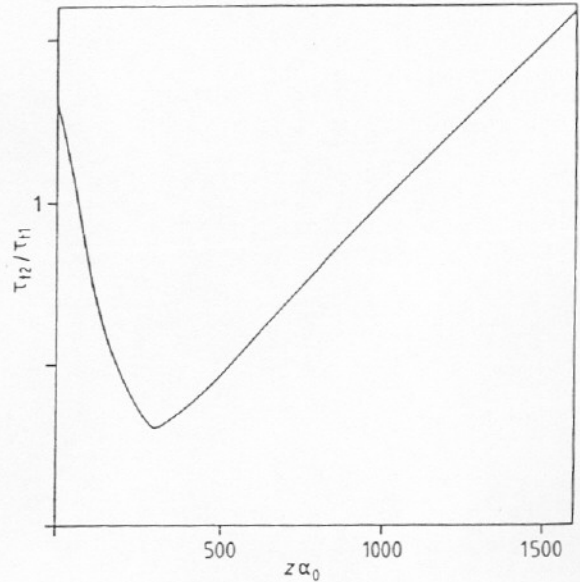


Figure 4. Plots of τ_{12}/τ_{11} against z_0/a_0 when $\alpha_1 = 23$ nm and $k_F a_0 = 0.0125$.

significant occupancy has taken place (see figure 3). We see that, when d is small $\tau_{s2}/\tau_{s1} < 1$. Then it increases rapidly to become greater than one for larger values of d . Thus, when $k_F a_0$ is in the region of 0.013, the values of τ_{s2}/τ_{s1} observed experimentally are consistent with the values of $d = 450$ which is in the order of the value it has in the experimental sample.

In figure 2 we plot the single-particle relaxation times τ_{s1} and τ_{s2} versus $k_F a_0$ and $d = 450$. We see that τ_{s2} (broken curve) rapidly becomes larger than τ_{s1} (full curve). We also see a small decrease in τ_{s1} immediately after the population of the second subband due to the (relatively small) intersubband scattering. After that τ_{s1} increases faster than before. Smith *et al* measure τ_{s1} when the occupation of the second subband is fairly large. The electron concentration of the first subband n_{s1} is only nine times larger than that of the second subband n_{s2} . They find that τ_{s1} is 1.7 times the value observed before the second subband is occupied. This is consistent with the behaviour of τ_{s1} exhibited in figure 2.

In figure 3 we plot the ratio τ_{12}/τ_{11} against d for the same parameter values as in figure 1. The behaviour of the scattering time ratio is different from that of the ratio of the single-particle relaxation times. We see that for small k_F the ratio is smaller than one even for large d . This means that there is a range of k_F where τ_{12} is always smaller than τ_{11} . For larger values of k_F we observe a similar behaviour to that shown in figure 1. This is in qualitative agreement with the experimental data (Van Houten *et al* 1988, Fang *et al* 1988).

In figure 4 we plot the ratio τ_{12}/τ_{11} against the spacer layer thickness z_0 for $\alpha_1 = 23$ nm and $k_F a_0 = 0.0125$. We see that, for small z_0 , τ_{12}/τ_{11} is larger than one. It decreases to a minimum value of 0.30 when $z_0/a_0 = 300$ and then it increases again.

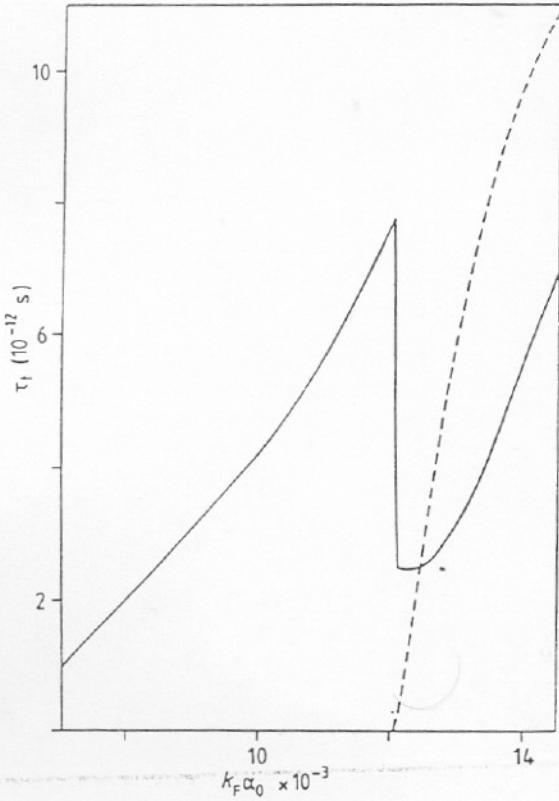


Figure 5. Plot of τ_{t1} (full curve) and (broken curve) against $k_F a_0$ when $d = 450$ and $z_0 = 1.5$ nm.

There are three significant factors that determine τ_{t2}/τ_{t1} . Firstly, there is the ratio of n_{s2}/n_{s1} which is always less than one: if we only take account of screening by the electrons in each subband (and ignore those in the other subbands) then τ_{t2}/τ_{t1} will be less than one when n_{s2}/n_{s1} is < 1 . The second factor is due to the difference of the mean distances between the impurities and the electrons in the subbands. When the impurities are near the interface this difference is many times bigger than the spacer layer thickness and is the dominant factor forcing the ratio τ_{t2}/τ_{t1} to values greater than one. When the impurities are well away from the interface the ratio of the mean distances of the impurities and the electrons in the second and first subbands tends to one and this factor begins to be less important. Then the main factor is the ratio n_{s2}/n_{s1} and τ_{t2}/τ_{t1} falls off with n_{s2}/n_{s1} as shown in figure 3. The third factor is the fact that the mean position of the electrons in the first subband lies between that for the second subband and the impurities. Consequently, the first-subband electrons screen the impurities very efficiently from the electrons in the second subband. When the impurities are remote from the electrons this additional screening becomes the dominant factor and leads to an increase in the ratio of τ_{t2}/τ_{t1} .

In figure 5 we plot τ_{t1} and τ_{t2} against $k_F a_0$ for the same parameter values as in figure 2. We find a large discontinuity in τ_{t1} and an increase in τ_{t1} after the population of the second subband with an initial rate similar to that before occupancy. This behaviour is completely different from that exhibited by τ_{s1} in figure 2. The main reason is the factor $(1 - \cos \theta)$ in the integrand in equation (18). After the population of the second subband when $n_{s2} \ll n_{s1}$, equation (17) becomes

$$\tau_{ti} = 1/P_i \quad (20)$$

because of approximate cancellation of all the other terms. This equation is similar to (15) except for the factor $(1 - \cos \theta)$ in the integrand. We see that there is a narrow range of k_F in which τ_{t2} is smaller than τ_{t1} . This range is very sensitive to d and z_0 (see

figures 3 and 4). In their work, Fang *et al* have assumed the occupancy of the second subband and found that $\tau_{12} > \tau_{11}$ as we would expect (Fang *et al* 1988). It would appear that Van Houten *et al* are working with much smaller values of n_{s2} , so that $\tau_{11} < \tau_{12}$ (Van Houten *et al* 1988).

5. Conclusion

Our calculations are in qualitative agreement with experimental data. The scattering time of the second subband τ_{12} is sometimes smaller and sometimes larger than τ_{11} (depending on the spacer layer thickness and the difference between the subbands widths). We find $\tau_{s2} = 2 \tau_{s1}$ in comparison with the experimental results $\tau_{s2} = 3 \tau_{s1}$ (Fang *et al* 1988) and $\tau_{s2} = 2.2 \tau_{s1}$ (Smith and Fang 1988).

The reason for these peculiar relationships between τ_t and τ_s is the rapid broadening of the spatial width of the subband wavefunction with increasing energy. We have used sinusoidal wavefunctions to bring out the essential physics of the problem in a simple way. For a more qualitative study of the problem it would be necessary to calculate more accurately the subband structure for each particular heterojunction and use variational wavefunctions instead of sinusoidal ones (Mori and Ando 1980).

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