Theory of quantum wells in external electric fields

1989 J. Phys.: Condens. Matter 1 4339

(http://iopscience.iop.org/0953-8984/1/27/006)

J. Phys.: Condens. Matter **1** (1989) 4339–4351. Printed in the UK

Theory of quantum wells in external electric fields

D P Barrio†, M L Glasser‡, V R Velasco† and F García-Moliner†

† Instituto de Ciencia de Materiales, CSIC, Serrano 123, 28006 Madrid, Spain

‡ Department of Mathematics and Computer Science, Clarkson University, Potsdam, NY 13676, USA

Received 31 October 1988, in final form 16 January 1989

Abstract. The theory of a rectangular quantum well in an external electric field is formulated in terms of surface Green function matching. This yields both the Green function and the wavefunction, and provides a practical method for the calculation of physical properties. The limits of validity of the equivalent-infinite-well approximation are studied. Applications to finite wells include the analysis of experimental data on the Stark shift of exciton peaks and quenching of the photoluminescence by the external field. The importance of an accurate estimate of the wavefunction for the electro-optical properties is stressed and demonstrated in practical terms.

1. Introduction

Fuelled by the growing interest in quantum well phenomena for semiconductor heterostructures there has been a renewed effort to understand the quantum mechanics of these systems on the basis of simple models. Basically, the calculation concerns the problem of matching at two inter-dependent interfaces; this is also true if the intermediate material is a barrier.

The purpose of this paper is to propose a matching technique that yields the Green function (GF) of the system and, on the basis of this technique, a practical method for performing calculations. The problem of a quantum well in an external electric field is also taken up. Section 2 presents the formal analysis leading to the secular equation. Section 3 contains an assessment of the limits of validity of the infinite-barrier approximation, while § 4 contains some examples of practical applications to the analysis of Stark shifts of excitonic peaks and to the quenching of the photoluminescence by the external electric field. The latter is more sensitive to the accuracy of the calculation, as it involves explicitly the field-dependent wavefunctions. Some conclusions are presented in § 5.

2. Surface GF matching analysis for a quantum well

Consider a composite system of the form A–L–B–R–C. Let G_j ($j = 1, 2, 3$ in correspondence with A, B, C) be the GF for infinite medium j. We concentrate on the layer B (G_2) and define the sum of the left (L) and right (R) interfaces as the projection domain. We want to construct the GF, G_s, of the system under study, starting from G_1, G_2, G_3,

0953-8984/89/274339 + 13 $02.50

which are presumed to be known. A given G is a function of two position-in-space arguments (x, x'). Let G_{L} denote that $x_3 = x_3' = x_3(\mathrm{L})$, $G_{\mathrm{L},\mu}$ that $x_3 = x_3(\mathrm{L})$, $x_3' = x_3(\mathrm{R})$ etc. Then define the 2×2 matrix projections

$$\mathbf{G}_2 = \begin{bmatrix} G_{2,\mathrm{L}} & G_{2,\mathrm{LR}} \\ G_{2,\mathrm{RL}} & G_{2,\mathrm{R}} \end{bmatrix} \qquad \mathbf{G}_2^{-1}\mathbf{G}_2 = \begin{bmatrix} \mathrm{L} & 0 \\ 0 & \mathrm{R} \end{bmatrix} = \mathbf{I} \tag{1}$$

and likewise for G_{s} and G_{s}^{-1}. Let P_j denote the projector onto the part of the space that is occupied by the material having GF G_j. We define the external projector $P_{\mathrm{e}} = P_1 + P_3$. The complete G_{s} can be related to its own projection G_{s} in exactly the same manner as for a general ABC sandwich formed from discrete media (Garcia-Moliner and Velasco 1986b, c):

$$\begin{aligned} P_2 G_{\mathrm{s}} P_2 &= P_2 G_2 P_2 + P_2 G_2 \mathbf{G}_2^{-1}(\mathbf{G}_{\mathrm{s}} - \mathbf{G}_2)\mathbf{G}_2^{-1} G_2 P_2 \\ P_{\mathrm{e}} G_{\mathrm{s}} P_2 &= P_{\mathrm{e}} G_{\mathrm{e}} \mathbf{G}_{\mathrm{e}}^{-1} \mathbf{G}_{\mathrm{s}} \mathbf{G}_2^{-1} G_2 P_2 \end{aligned} \tag{2}$$

where

$$P_{\mathrm{e}} G_{\mathrm{e}} P_{\mathrm{e}} = P_1 G_1 P_1 + P_3 G_3 P_3 \qquad \mathbf{G}_{\mathrm{e}} = \begin{bmatrix} G_{1,\mathrm{L}} & 0 \\ 0 & G_{3,\mathrm{R}} \end{bmatrix}. \tag{3}$$

There is a dual set of formulae with e and 2 interchanged. From the diagonal parts of G_{s} one can calculate the spectral functions of interest, e.g. total or local density of states, while the secular equation for the well modes is

$$\det \mathbf{G}_{\mathrm{s}}^{-1} = 0. \tag{4}$$

Here Fourier transforms parallel to the interfaces are understood to be taken, so G_{s} is a function of (κ, E). The problem is reduced to finding G_{s} and in this lies the difference between discrete and continuous media.

In terms of wavefunctions, having matched ψ—which ensures continuity of the probability density—one must in general match $m^{-1}\psi'$, thus ensuring continuity of the current density. On going over to GF matching this results in the matching of $G(x_3, x_3')$ and $m^{-1\prime}G(x_3, x_3')$, where x_3 is the spatial coordinate normal to the interfaces and the prime preceding G denotes differentiation with respect to the first argument. Expressing the matching condition at the L and R interfaces and proceeding as in García-Moliner and Velasco (1986a), we find

$$\mathbf{G}_2^{-1} = -\frac{\hbar^2}{2}\begin{bmatrix} B_{\mathrm{LL}} & B_{\mathrm{LR}} \\ B_{\mathrm{RL}} & B_{\mathrm{RR}} \end{bmatrix} \tag{5}$$

where, taking $x_3 = 0, L$ for the L, R interfaces—so L is the well thickness—we have

$$\begin{aligned} B_{\mathrm{LL}} &= (m_1^{-1\prime}\mathcal{G}_1^{(+)}\mathcal{G}_1^{-1} - m_2^{-1\prime}\mathcal{G}_2^{(-)}\mathcal{G}_2^{-1})_{\mathrm{L}}\mathcal{G}_2(0) \\ B_{\mathrm{LR}} &= (m_1^{-1\prime}\mathcal{G}_1^{(+)}\mathcal{G}_1^{-1} - m_2^{-1\prime}\mathcal{G}_2^{(+)}\mathcal{G}_2^{-1})_{\mathrm{L}}\mathcal{G}_2(0, L) \\ B_{\mathrm{RL}} &= (m_2^{-1\prime}\mathcal{G}_2^{(-)}\mathcal{G}_2^{-1} - m_3^{-1\prime}\mathcal{G}_3^{(-)}\mathcal{G}_3^{-1})_{\mathrm{R}}\mathcal{G}_2(L, 0) \\ B_{\mathrm{RR}} &= (m_2^{-1\prime}\mathcal{G}_2^{(+)}\mathcal{G}_2^{-1} - m_3^{-1\prime}\mathcal{G}_3^{(-)}\mathcal{G}_3^{-1})_{\mathrm{R}}\mathcal{G}_3(L) \end{aligned} \tag{6}$$

where

$$'\mathcal{G}_j^{(\pm)} = \lim_{x_3' \to x_3 \pm 0} \frac{\partial \mathcal{G}}{\partial x_3}(x_3, x_3'). \tag{7}$$

The secular equation is then

$$B_{LL}B_{RR} - B_{LR}B_{RL} = 0. \tag{8}$$

This yields the eigenvalues for an arbitrary quantum well, where A and C need not be the same.

The signs and factors in (5) are in accordance with the following convention: let $\mathcal{H}_j$ be the Hamiltonian of medium j

$$\mathcal{H}_j = -(\hbar^2/2m_j)\nabla^2 + V_j(x_3) \tag{9}$$

then

$$(EI - \mathcal{H}_j)G_j = \delta(x_3 - x_3'). \tag{10}$$

After Fourier transform parallel to the interfaces, E is actually to be understood as $E + \hbar^2\kappa^2/2m_j$. With this convention the discontinuity in the normal derivative is

$${}'\mathcal{G}_j^{(+)} - {}'\mathcal{G}_j^{(-)} = -2m_j/\hbar^2. \tag{11}$$

In practice we shall be interested in the ground level ($\kappa = 0$) of the energy sub-bands for the quantum well, so we shall simply write E.

The description of the barriers for $x_3 < 0$ and $x_3 > L$ involves the question of the boundary conditions away from the well. An electric field from $-\infty$ to $+\infty$ would correspond to incoming flux at one end and outgoing flux at the other end and this does not actually correspond to the experimental arrangement, in which there is no charge flow through the sample. In the calculations for these systems it is customary to eliminate the electric field from the asymptotic limits by putting either constant potentials or infinite barriers at $x_3 = -D$ and $x_3 = L + D$, where D is a conveniently large distance. This keeps the electric field outside the well but allows a calculation in terms of stationary states, i.e. real eigenvalues. In fact the results do not show any significant difference if the field outside the well is omitted altogether—this has been checked here for fields attained in actual experiments—unless one is explicitly interested in lifetime effects, which are outside the scope of this paper. Thus for an electric field $\mathcal{E}$ exerting a force, $F = e\mathcal{E}$ on the electron, we shall define the outside potential to be a constant equal to V_1 for $x_3 \leqslant 0$ and to $V_1 + FL$ for $x_3 \geqslant L$. There is no difficulty in including the field outside, but this complication is really unnecessary for the issues we wish to discuss.

In order to carry out the operations indicated in (4)–(6) it is necessary to know the Gs involved. For regions 1 and 3 we simply use the GF of a free particle of mass m_1 in a constant potential, with $V_3 = V_1 + FL$, as explained. G_2 is discussed in the Appendix. Using either (A8) or (A10) we obtain the secular equation

$$\begin{aligned}\{K - [(aF)^{1/3}/m_2]C_2'(z_0)/C_2(z_0)\}\{K + [(aF)^{1/3}/m_2]C_1'(z_L)/C_1(z_L)\}C_2(z_0)C_1(z_L)\\ = \{K - [(aF)^{1/3}/m_2]C_1'(z_0)/C_1(z_0)\}\\ \times \{K + [(aF)^{1/3}/m_2]C_2'(z_L)/C_2(z_L)\}C_1(z_0)C_2(z_L)\end{aligned} \tag{12}$$

where, selecting the energy origin in such a way that $V_1(x_3 = 0) = 0$ and $V_2(x_3 = 0) = U_0$,

$$\begin{aligned} K &= (2|E|/m_1\hbar^2)^{1/2} & z_0 &= -(aF)^{1/3}(U_0 - |E|)/F \\ z_L &= (aF)^{1/3}[L - U_0 - |E|)/F] & a &= 2m_2/\hbar^2. \end{aligned} \tag{13}$$

At this point it is convenient to introduce the dimensionless parameters

$$\varepsilon = |E|/U_0 \qquad y = 2m_2U_0L^2/\hbar^2$$
$$\alpha = m_2/m_1 \qquad u = FL/U_0 \tag{14}$$

where U_0 is the barrier height, i.e., $V_1 - V_2$ at $x_3 = 0$. Then (12) simplifies to

$$[(\alpha\varepsilon y)^{1/2} - (uy)^{1/3}F_1(z_0)][(\alpha\varepsilon y)^{1/2} + (uy)^{1/3}F_1^*(z_L)]$$
$$= [(\alpha\varepsilon y)^{1/2} - (uy)^{1/3}F_1^*(z_0)][(\alpha\varepsilon y)^{1/2} + (uy)^{1/3}F_1(z_L)]F_2(z_0)F_2^*(z_L) \tag{15}$$

where

$$F_1(z) = (\mathrm{Ai}(z)\mathrm{Ai}'(z) + \mathrm{Bi}(z)\mathrm{Bi}'(z) + \mathrm{i}\pi^{-1})/(\mathrm{Ai}^2(z) + \mathrm{Bi}^2(z))$$
$$= (uy)^{1/3}(f_1(z) + \mathrm{i}f_2(z)) \tag{16}$$
$$F_2(z) = [2\mathrm{Ai}(z)\mathrm{Bi}(z) + \mathrm{i}(\mathrm{Ai}^2(z) - \mathrm{Bi}^2(z))]/(\mathrm{Ai}^2(z) + \mathrm{Bi}^2(z))$$
$$= g_1(z) + \mathrm{i}g_2(z).$$

Finally, with $\lambda_\pm(z) = (\alpha\varepsilon y)^{1/2} \pm f_1(z)$, the real part of (15) becomes

$$(\lambda_-(z_0)\lambda_+(z_L) - f_2(z_0)f_2(z_L))(1 - g_1(z_0)g_1(z_L) - g_2(z_0)g_2(z_L))$$
$$- (\lambda_-(z_0)f_2(z_L) + \lambda_+(z_L)f_2(z_0))(g_1(z_0)g_2(z_L)$$
$$- g_1(z_L)g_2(z_0)) = 0. \tag{17}$$

Because $g_1^2(z) + g_2^2(z) = 1$, the imaginary part of (15) is equivalent to (17).

In the zero-field limit,

$$z_0 = -(uy)^{1/3}(1 - \varepsilon)/u \qquad z_L = (uy)^{1/3}(u + \varepsilon - 1)/u \tag{18}$$

both become large and negative (since in our case $0 < \varepsilon < 1$). By utilising the asymptotic behaviour of the Airy functions in this limit

$$\mathrm{Ai}(z) \sim \pi^{-1/2}|z|^{-1/4}\sin(\zeta + \pi/4)$$
$$\mathrm{Bi}(z) \sim \pi^{-1/2}|z|^{-1/4}\cos(\zeta + \pi/4) \qquad \zeta = 2/3|z|^{3/2} \tag{19}$$

we find that (17) becomes

$$[(\alpha - 1)\varepsilon - 1]\sin\{[(1 - \varepsilon)y]^{1/2}\} + 2[\alpha\varepsilon(1 - \varepsilon)^{1/2}]\cos\{[(1 - \varepsilon)y]\}^{1/2} = 0 \tag{20}$$

which, for $\alpha = 1$ is the well known transcendental equation for the bound states of a square well.

3. The infinite-barrier well

In order to simplify the calculation, a given quantum well of finite barrier height and thickness L is often replaced by a well with infinite barriers with some parameter adjusted so as to reproduce the zero-field ground state exactly. For zero field G_s vanishes and, if G is the GF of the medium inside the well, then it follows from (2) that the secular equation is

$$\det \mathbf{G} = 0. \tag{21}$$

Using either (A8) or (A9) this yields

$$\mathrm{Ai}(z_0')\mathrm{Bi}(z_L') - \mathrm{Ai}(z_L')\mathrm{Bi}(z_0') = 0 \tag{22}$$

where z_0' and z_L' are given by (A6) with $V = 0$. This equation was first derived independently by Trallero-Giner and López-Gondar (1986) and by Matsuura and Kamizato (1986). The former found that the equivalent infinite well can account for the experimental results of Wood *et al* (1984) and of Alibert *et al* (1985)—the Stark shift of excitonic peaks—if the effective mass of the carriers in the well is the adjustable parameter. All other authors choose to adjust the thickness of the well, which appears to be more intuitive. However, the point is that the first choice requires small mass changes, whereas it will presently be seen that replacing L by an 'equivalent' $L' > L$ leads in practice to impossibly high values of L'. The question of the accuracy of the results obtained with the fictitious equivalent infinite well has been discussed in detail (Fritz 1987). While it would seem that this approximation appears to be reasonable in practice, it is important to note that this analysis is based on fitting L' for *zero field* and then using this one value of L' for all $\mathscr{E} \neq 0$. Moreover, *only the eigenvalue* is studied, while the 'equivalent' well is often used as a simpler model using which one can study, say, optical absorption (Matsuura and Kamizato 1986, Ahn and Chuang 1987), for which one needs the *wavefunction*. At the very least one ought to find $L'(\mathscr{E})$ for each value of $\mathscr{E}$ if one expects to obtain a reasonable approximation for the wavefunction ψ, as the details of the dependence on $\mathscr{E}$ of ψ are very important for the electro-optical properties of the well.

Figure 1 shows the situation for the well used in the experiments of Wood *et al* (1984). The thicker curve gives the ground-state ($\kappa = 0$) eigenvalue of the lowest subband as a function of $\mathscr{E}$ for the finite well, calculated from (17). The family of thin curves give this eigenvalue for different values of L' using (22) for the 'equivalent' infinite well. The value of L' needed to fit the ground-state eigenvalue at each $\mathscr{E}$ is obtained from the intersections with the thin curves. The result is shown in figure 2. At zero field L' is very close to L, but as $\mathscr{E}$ increases L' increases very steeply until a critical value u_c is found, which requires $L' \to \infty$. In this case $u_c = 0.18$, while in the experiments values of u up to 0.31 were attained.

Figure 3 shows L'—or, rather $\Lambda = L'/L$—versus $\mathscr{E}$ for the cases studied by Fritz (1987), by Matsuura and Kamizato (1986) and by Ahn and Chuang (1987), while table 1 compares the corresponding values of u_c with the highest or typical fields attained in practice in the cases under study. It is clear that the simplification of the equivalent-infinite-well model involves very severe shortcomings in practice and that, especially where the dependence on $\mathscr{E}$ of ψ is important, it is necessary to do better in order to obtain the wavefunction. This will be discussed again in § 4.2.

4. Practical applications

We shall consider QWs in which the well material is GaAs and the barrier material is Al $\mathrm{Ga}_{1-x}\mathrm{As}$ for $x < 0.4$, i.e. a direct-gap material. The study will then be centred on vertical transitions between hole and electron states with $\kappa = 0$. In the effective-mass approximation for $\kappa = 0$, if $\boldsymbol{k}\cdot\boldsymbol{p}$ coupling between conduction and valence bands is neglected the bands may be decoupled for zincblende structure semiconductors (Altarelli 1985). This approximation, which is widely used, will also be used here. Practical experience shows that it yields the correct eigenvalues (Pérez-Alvarez *et al* 1988) to

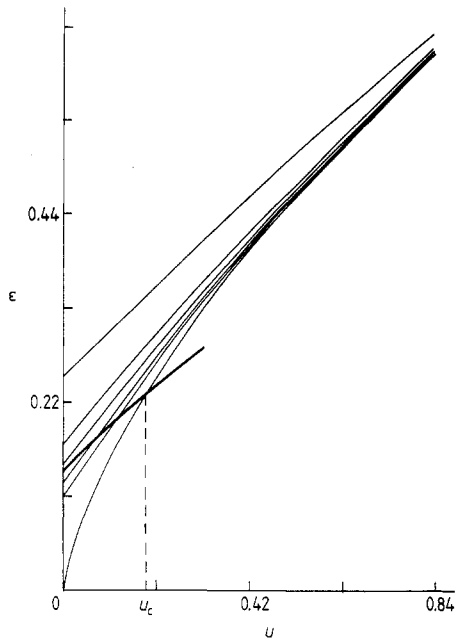

Figure 1. Thin curves: the field dependence of the ground state—lowest sub-band—for an infinite well with different values of L' ($\varepsilon = E/U_0$; $u = FL/U_0$). From top to bottom L' (nm) is 10, 12, 13, 14, 15, ∞. Thicker curve: the field dependence of the exact eigenvalue for the finite well. The example corresponds to the experiments of Wood *et al* (1984).

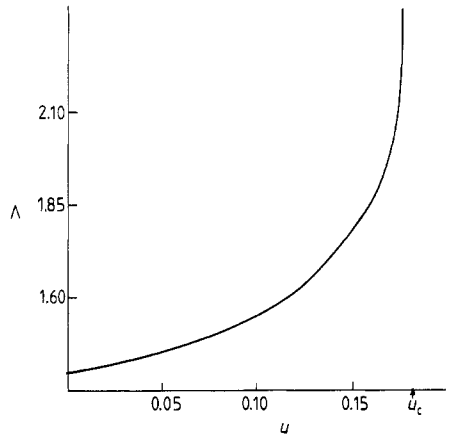

Figure 2. The information contained in figure 1 is cast as the dependence on $\mathscr{E}$ of $\Lambda = L'/L$, where L' is the fictitious thickness of the equivalent infinite well required to reproduce the $\mathscr{E}$-dependent eigenvalue.

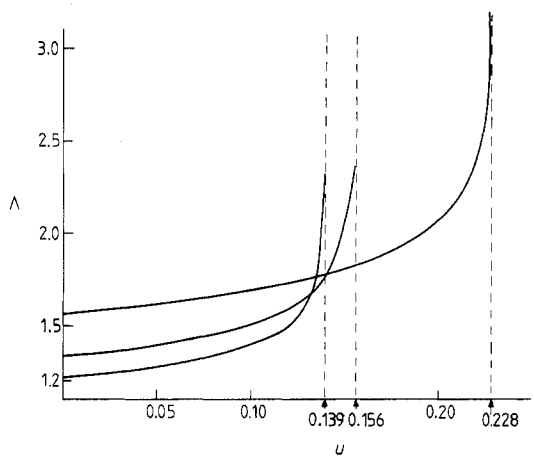

Figure 3. As figure 2 but for the three cases indicated in table 1.

Table 1. A comparison of u_c with the maximum or typical fields attained expressed as multiples of u in the second column and as multiples of $\mathscr{E}$ in the third column.

Critical value	Maximum attained (or typical) u	Corresponding $\mathscr{E}$ (kV cm^{-1})
0.228[a]	0.663[b]	250
0.156[c]	0.443[d]	65
0.139[e]	1.057[f]	35

[a] Ahn and Chuang (1987) [b] West and Eglash (1985)
[c] Matsuura and Kamizato (1986) [d] Yamanaka *et al* 1986
[e] Fritz (1987) [f] Fritz *et al* (1986).

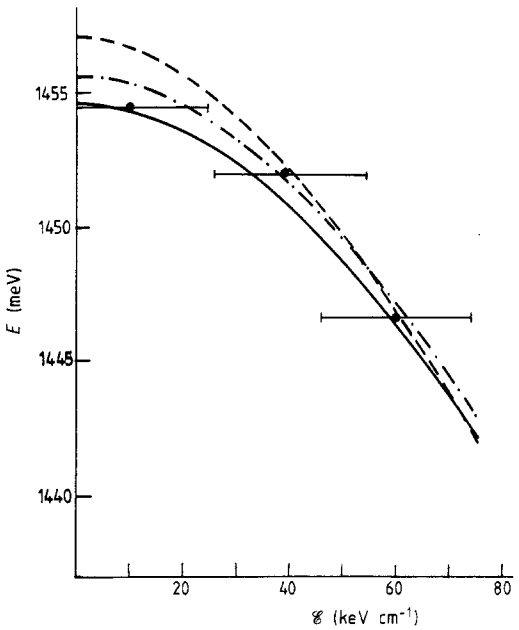

Figure 4. The Stark shift of the excitonic peak associated with the highest heavy hole and the lowest electron bands. Full circles: experimental results (Wood *et al* 1984). Broken, chain and full curves: results calculated with band offset rules A, B and C, respectively—see the text.

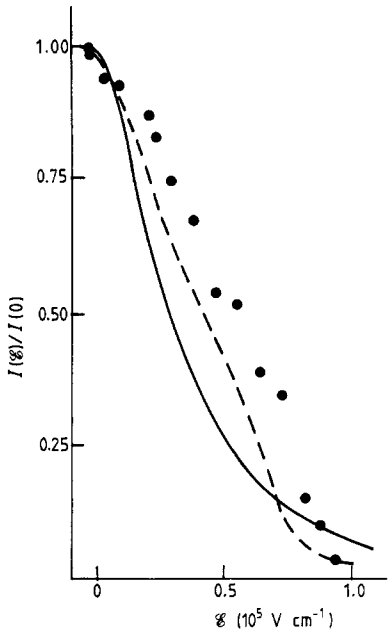

Figure 5. The integrated photoluminescence intensity versus electric field, normalised with respect to zero-field conditions. Full circles: results of the variational calculation of the overlap between electron and hole wavefunctions (Viña *et al* 1987). Broken curve: from present calculation.

an accuracy of a fraction of a meV compared with the results obtained with an eight-band model including remote-band effects to second order (Pötz and Ferry 1985).

For GaAs we use the effective masses commonly found in the literature ($m_e = 0.0665\, m_0$, $m_{lh} = 0.08\, m_0$, $m_{hh} = 0.45$). For heavy holes it has been suggested that one should take instead $m_{hh} = 0.34$ (Miller *et al* 1984). This will be considered presently. For the gap difference, which depends on x, we use the formula $\Delta E_g = (1155x + 370x^2)$ meV (Lee *et al* 1980). The question of the band offset rule has been abundantly discussed. Various proposals will be considered—see figure 4. Finally, for

the effective masses in the ternary compound we use (Xu *et al* 1983)

$$m_e(x) = (0.0665 + 0.0835x)m_e(0)$$
$$m_{lh}(x) = (0.08 + 0.057x)m_{lh}(0) \tag{23}$$
$$m_{hh}(x) = (0.45 + 0.302x)m_{hh}(0)$$

except that 0.45, for heavy holes, may be replaced by 0.34, as indicated.

4.1. The Stark shift of excitonic peaks

Figure 4 shows the experimental data of Wood *et al* (1984) for a QW for which L = 9.5 nm and $x = 0.32$. The curves were calculated from (17) by using the value of 8.3 meV for the exciton binding energy (Greene *et al* 1984) and neglecting its dependence on $\mathscr{E}$ (Brum and Bastard 1985). The three different curves, related to rules A, B, C, correspond to different proposals that have been made for the band offset. On these purely empirical grounds we shall adopt rule B (Wang *et al* 1984), i.e. the 65–35 rule, meaning that the band-edge discontinuity is 65% of the total ΔE_g for the conduction band. The results are very close to those obtained with rule C, i.e. the 57–43 rule (Miller *et al* 1984), the largest difference being of order 10^{-3}, and the same was found in other cases for which calculations were also performed. Yet another empirical rule for the band offset, namely the 62–38 rule, has been proposed by Watanabe *et al* (1985). It is clear that anything in the neighbourhood of 60–40 is reasonable, and that small differences are unimportant.

Table 2 shows the experimental results of Collins *et al* (1986) and the values calculated from (17) with the 65–35 band-offset rule and with the two values 0.45 and 0.34 for the heavy-hole effective mass. The second column gives the values of u for the hole well, which is much more sensitive than the electron well to the effect of the electric field. All transitions involve the lowest electron sub-band and the different hole bands indicated in the tables. Note that for the highest fields $u = 0.89$, which means a very high effective field, and still the agreement with experiment is quite good, with a maximum deviation of 3.6%. It is seen that the difference between the results obtained by using the two values for m_{hh} is essentially irrelevant.

4.2. The wavefunction: quenching of the photoluminescence

It is seen in the above examples that the eigenvalues can be obtained to a good accuracy from a simple model, in agreement with general experience. Finding the dependence on $\mathscr{E}$ of the wavefunction is a more difficult problem, but is very important for studies of many electro-optical properties. We shall consider the quenching of the photoluminescence of a quantum well by an external electric field. As $\mathscr{E}$ increases, the electron and hole wavefunctions have increasingly separate confinements and their overlap decreases. The quenching of the photoluminescence is essentially due to this and thus the dependence on $\mathscr{E}$ of the wavefunction is important.

The wavefunction $\psi_s(x_3)$ of a bound state of the quantum well can be obtained once $G_s(x_3, x_3')$ is known, by taking residues in (2). Let ψ_s be the two-component vector

$$\{\boldsymbol{\psi}_L = \psi_s(0), \boldsymbol{\psi}_R = \psi_s(L)\}$$

remembering that $z = 0/L$ for the L/R interfaces, and put

$$\mathbf{G}_s^{-1} = \boldsymbol{\Gamma}_s = \begin{bmatrix} \Gamma_{s,LL} & \Gamma_{s,LR} \\ \Gamma_{s,RL} & \Gamma_{s,RR} \end{bmatrix} \qquad \mathbf{G}_2^{-1} = \boldsymbol{\Gamma}_2 = \begin{bmatrix} \Gamma_{2,LL} & \Gamma_{2,LR} \\ \Gamma_{2,RL} & \Gamma_{2,RR} \end{bmatrix}. \tag{24}$$

Table 2. The position of the excitonic peak versus applied electric field. First column: $\mathscr{E}$. Second column: Equivalent dimensionless strength $u = FL/U_0$. The experimental data are from Collins *et al* (1986). The transitions studied involve the lowest electron sub-band and the hole sub-bands indicated at the top. The figures in brackets below the calculated values give the fractional deviation $[(E_{calc} - E_{expt})/E_{expt}] \times 100$.

		1-hh			2-hh		
$\mathscr{E}$ (10^4 V cm^{-1})	$u(h)$	Calc.†	Expt	Calc.‡	Calc.†	Expt	Calc.‡
4.86	0.26	1554 (0.1)	1553	1552 (−0.1)	1588 (−0.3)	1593	1580 (−0.8)
6.29	0.33	1552 (0.3)	1548	1550 (0.1)	1588 (−0.3)	1592	1580 (−0.8)
7.24	0.38	1550 (0.4)	1544	1548 (0.2)	1587 (−0.3)	1592	1580 (−0.8)
8.43	0.44	1548 (0.6)	1539	1545 (0.4)	1587 (−0.3)	1591	1579 (−0.8)
9.62	0.50	1545 (0.8)	1533	1542 (0.6)	1586 (−0.3)	1590	1578 (−0.8)
12.00	0.68	1538 (1.3)	1518	1535 (1.1)	1584 (0.1)	1581	1576 (−0.3)
14.38	0.75	1530 (2.0)	1500	1527 (1.8)	1581 (0.8)	1568	1572 (0.3)
16.76	0.87	1522 (2.8)	1480	1518 (2.6)	1577 (1.3)	1557	1568 (0.8)
19.14	0.89	1513 (3.6)	1460	1509 (3.4)	1573 (1.7)	1546	1563 (1.1)

		3-hh			1-lh	
$\mathscr{E}$ (10^4 V cm^{-1})	$u(h)$	Calc.†	Expt	Calc.‡	Expt	Calc.
4.86	0.26				1572	1576 (0.2)
6.29	0.33	1636 (−0.7)	1648	1620 (−1.7)	1568	1574 (0.4)
7.24	0.38	1636 (−0.7)	1647	1619 (−1.7)	1564	1573 (0.6)
8.43	0.44	1635 (−0.6)	1645	1619 (−1.6)	1560	1571 (0.7)
9.62	0.50				1554	1569 (1.0)
12.00	0.68				1542	1564 (1.4)
14.38	0.75				1528	1558 (2.0)
16.76	0.87				1508	1551 (2.9)
19.14	0.89				1490	1543 (3.6)

† $m_{hh} = 0.34\, m_0$.
‡ $m_{hh} = 0.45\, m_0$.

Taking residues in (2) for $x_3 \leqslant 0$:

$$\psi_s(x_3) = G_1(x_3, 0)G_{1L}^{-1}\boldsymbol{\psi}_L \qquad (x_3 \leqslant 0) \tag{25}$$

where $G_{1L} = G_1(0, 0)$. Now take residues in (2) for $0 \leqslant x_3 \leqslant L$ and note that (4) is the secular determinant of the matching equations

$$\begin{bmatrix} \Gamma_{s,LL} & \Gamma_{s,LR} \\ \Gamma_{s,RL} & \Gamma_{s,RR} \end{bmatrix} \begin{bmatrix} \boldsymbol{\psi}_L \\ \boldsymbol{\psi}_R \end{bmatrix} = 0. \tag{26}$$

Then

$$\psi_s(x_3) = [G_2(x_3, 0), G_2(x_3, L)] \begin{bmatrix} \Gamma_{2,LL} & \Gamma_{2,LR} \\ \Gamma_{2,RL} & \Gamma_{2,RR} \end{bmatrix} \begin{bmatrix} \boldsymbol{\psi}_L \\ \boldsymbol{\psi}_R \end{bmatrix} = 0 \qquad (0 \leqslant x_3 \leqslant L) \tag{27}$$

while

$$\psi_s(x_3) = G_3(x_3, L)G_{3R}^{-1}\boldsymbol{\psi}_R \qquad (x_3 \geqslant L). \tag{28}$$

Note that $V_3 \neq V_1$ and thus $G_3 \neq G_1$. Now, from (28):

$$\boldsymbol{\psi}_R = -[\Gamma_{s,RR}]^{-1}\Gamma_{s,RL}\boldsymbol{\psi}_L \tag{29}$$

and using this in (27) and (28) the wavefunction $\psi_s(x_3)$ is cast for all x_3 in terms of only one amplitude, namely ψ_L. The information on the matching is contained in all the GF entering (25), (27) and (28), evaluated at the energy eigenvalue obtained from (4). The amplitude is obtained by normalisation—note that this depends also on $\mathscr{E}$—and thus the normalised wavefunctions for the electron and hole states involved in the transition under study are obtained exactly as functions of $\mathscr{E}$. Then the overlap

$$|M_{eh}|^2 = \left| \int dx_3 \; \psi_e^*(x_3) \; \psi_h(x_3) \right|^2 \tag{30}$$

can be evaluated as a function of $\mathscr{E}$ and compared with experimental data on the integrated photoluminescence intensity versus electric field. Figure 5 gives the results of such a calculation compared with those of a variational calculation and with the experimental data of Viña *et al* (1987), showing a definite improvement upon the variational calculation and a fairly good agreement with experiment—see the comments later.

5. Conclusions

We have demonstrated the practical use of the surface GF matching analysis in studying quantum wells in external electric fields. The main factor, unless one is explicitly interested in lifetime effects, is the linear variation of the potential inside the well. However, the same analysis can be equally extended to include the electric field outside. One then has quasi-stationary states with complex eigenvalues $(E_r + iE_i)$. We have performed some sample calculations and found that fractional deviations of E (stationary, real) from E_r are typically of order 10^{-3} and in extreme cases of order 10^{-2}, no larger than the orders of magnitude given in brackets in table 2. These findings agree with results obtained from transfer-matrix calculations (Lago and Pérez-Alvarez 1988).

An analysis in terms of quasi-stationary states would be necessary in order to study

lifetime effects explicitly, as seen above for the high-field end of figure 5, but it proves unnecessary in practice for studying energy levels. In this context a remark concerning the basis of the theoretical approach is appropriate. Recently Austin and Jaros (1985, 1987, 1988) have clarified an apparent discrepancy from the work of Ahn and Chuang (1986) for high fields. The former authors use a scattering theoretic approach centred on the concept of phase shift, while the latter formulate the problem in terms of Airy functions of complex arguments. As stressed by Austin and Jaros (1988), the two approaches are complementary and the results are equivalent. Moreover, for some problems the scattering theoretic approach is the obvious one. These views are completely in line with those of the present work. On one hand, the GF matching can be identically cast as wavefunction matching, as demonstrated in § 4.2. The results of Lago and Pérez-Alvarez (1988), which also agree with ours, were actually obtained by working with Airy functions of complex argument. On the other hand the GF, the propagator, is a central concept in scattering theory. The very formal derivation of the surface GF matching analysis is scattering theoretic. Its relationship to the phase-shift analysis has also been discussed elsewhere (García-Moliner and Flores 1979, Dobrzynski *et al* 1987).

Once the GF G_s of the system is known one can obtain from it all desired physical quantities. In particular we have stressed the importance of obtaining a good estimate of the wavefunction, which can also be readily obtained from G_s, and which is related to the electro-optical properties. The frequently made approximation of replacing the actual well of thickness L by an equivalent infinite well of thickness L' could not produce a good approximation to ψ, as discussed in § 2. The calculation of the electron–hole overlap compares very well with experimental data on quenching of the photoluminescence by the external field and improves considerably upon the results based on a variational determination of ψ, as was to be expected. Of course this is only a test of the quality of the wavefunction, not a complete theory of the quenching of the photoluminescence, as lifetime effects have not been included and these should dominate for sufficiently high fields. In fact Köhler *et al* (1988) find, for a well that is fairly similar in composition and thickness, that this happens beyond about 80 kV cm^{-1}, which checks with the situation seen in figure 5. We also note that the experiments analysed here were performed with samples consisting of five wells and it has been suggested (McIlroy 1986) that the results may differ considerably from those obtained for a single well. There would be no difficulty in doing the calculation for a MQW. Having found the GF for one well one can easily relate it to the transfer matrix (Pérez-Alvarez *et al* 1988) and then treat any desired number of wells directly. However, the results shown in figure 5 would not lead one to expect any large differences. The findings of McIlroy (1986) could be different because of the very small value—2.5 nm—of the well thickness employed. In fact McIlroy repeated the calculations for $L =$ 7.5 nm and then found the effects much less pronounced. In this context it is interesting to note some recent experiments (Mendez *et al* 1988) where well coupling effects are studied from low to high fields, again with narrow wells −3.0 nm well thickness, 3.5 nm barrier thickness in a GaAs–$Ga_{0.65}Al_{0.35}As$ superlattice—leading to the formation of Stark ladders and associated phenomena. This is an interesting problem for further study.

In conclusion we have demonstrated the practical use of the surface GF matching analysis to study quantum wells in external electric fields. The same method could be used with equal ease to study other problems, e.g. tunnelling across a barrier.

Acknowledgments

This work was partially supported by the Spanish Comisión Asesora de Investigación Científica y Técnica, grant 94-84. MLG wishes to thank the US–Spain Joint Committee for Scientific and Technological Cooperation for a travel grant to the CSIC in Madrid where this work was initiated. The authors thank R Pérez-Alvarez for many stimulating discussions and for information on his current work.

Appendix. The electric-field-dependent Green function

Consider the one-electron Hamiltonian

$$\mathcal{H} = p^2/2m + Fx_3 + V \tag{A1}$$

where V and $F > 0$ are constant. By translational symmetry the solution to

$$[-(\hbar/2m)\,\mathrm{d}^2/\mathrm{d}x_3^2 + Fx_3 + V - E]\varphi_E(x_3) = 0 \tag{A2}$$

is

$$\varphi_E(x_3) = \varphi_0(x_3 - E/F). \tag{A3}$$

In terms of the variable

$$\xi = (2mF/\hbar^2)^{1/3}(x_3 + V/F) \tag{A4}$$

φ_0 satisfies the Airy equation

$$y'' - \xi y(\xi) = 0. \tag{A5}$$

Therefore, $\varphi_E(x_3)$ is a linear combination of the Airy functions $\mathrm{Ai}(z)$, $\mathrm{Bi}(z)$ with

$$z = (2mF/\hbar^2)^{1/3}[x_3 + (V - E)/F] \tag{A6}$$

and the GF corresponding to (A1) has the form

$$G(x_3x_3';E) = N\begin{cases}(a_1\mathrm{Ai}(z) + \mathrm{Bi}(z))(a_1'\mathrm{Ai}(z') + \mathrm{Bi}(z')) & x_3 \geqslant x_3' \\ (a_2\mathrm{Ai}(z) + \mathrm{Bi}(z))(a_2'\mathrm{Ai}(z') + \mathrm{Bi}(z')) & x_3 \leqslant x_3'\end{cases} \tag{A7}$$

where the constants are determined by continuity and the jump condition. In addition we require that (A7) possess the proper zero-field limit. The unique solution satisfying these requirements is, with our sign conventions,

$$G(x_3, x_3') = \frac{\pi a}{2(aF)^{1/3}}\begin{cases}C_1(z)C_2(z') & x_3 \geqslant x_3' \\ C_1(z')C_2(z) & x_3 \leqslant x_3'\end{cases} \tag{A8}$$

where $a = 2m_2/\hbar^2$ and

$$C_1(z) = \mathrm{Ai}(z) - \mathrm{iBi}(z) \qquad C_2(z) = \mathrm{Bi}(z) - \mathrm{iAi}(z) = -\mathrm{i}C_1^*(z). \tag{A9}$$

To our knowledge, equation (A8) has not appeared in the literature before. However, equivalent GF satisfying other boundary conditions are known (Moyer 1973, Davison and Kolar 1985, Davison *et al* 1980).

The question of which boundary conditions should be used outside the well is discussed in the text. The main question concerns the well region, for which (A8) is

the G for an electric field $\mathscr{E}$ exerting on the electron a force $F = e\mathscr{E}$ in the positive direction. However, this corresponds to an infinite medium with the said electric field. In fact, provided the field is the correct one inside the well, the boundary conditions at the L and R interfaces are arbitrary (Pérez-Alvarez *et al* 1988). The simplest G one can write down is actually

$$G_2(x_3, x_3') = \frac{\pi_a}{(aF)^{1/3}} \begin{cases} \mathrm{Ai}(z)\,\mathrm{Bi}(z') & x_3 \geqslant x_3' \\ \mathrm{Ai}(z')\,\mathrm{Bi}(z) & x_3 \leqslant x_3' \end{cases} \tag{A10}$$

which can be equally appropriately used with evident economy of algebra. In fact it is easily verified that (A10) and (A8) yield the same secular equation (12), as they must.

References

Ahn D and Chuang S L 1986 *Phys. Rev.* B **34** 9034
—— 1987 *Phys. Rev.* B **35** 4149
Alibert C, Gaillard S, Brum J A, Bastard G, Frijlink P and Erman M 1985 *Solid State Commun.* **54** 457
Altarelli M 1985 *J. Lumin.* **30** 472
Austin E J and Jaros M 1985 *Phys. Rev.* B **31** 5569
—— 1987 *J. Appl. Phys.* **62** 558
—— 1988 *Phys. Rev.* B **38** 6326
Brum J A and Bastard G 1985 *Phys. Rev.* B **31** 3893
Collins R T, von Klitzing K and Ploog K 1986 *Phys. Rev.* B **33** 4378
Davison S G and Kolar M 1985 *J. Phys. C: Solid State Phys.* **18** 4581
Davison S G, Ueba H and Jerrard R J 1980 *J. Phys. C: Solid State Phys.* **13** 1351
Dobrzynski L, Velasco V R and García-Moliner F 1987 *Phys. Rev.* B **35** 5872
Fritz I J 1987 *J. Appl. Phys.* **55** 2273
Fritz I J, Doyle B L, Drummond T J, Biefeld R M and Osbourn G C 1986 *Appl. Phys. Lett.* **48** 1606
García-Moliner F and Flores F 1979 *Introduction to the Theory of Solid Surfaces* (Cambridge: CUP)
García-Moliner F and Velasco V R 1986a *Surf. Sci.* **17** 9
—— 1986b *Prog. Surf. Sci.* **21** 93
—— 1986c *Phys. Scr.* **34** 252
Greene R L, Bajaj K K and Phelps D E 1984 *Phys. Rev.* B **29** 1807
Köhler K, Polland H-J, Schultheis L and Tu C W 1988 *Phys. Rev.* B **38** 5496
Lago M and Pérez-Alvarez R 1988 private communication
Lee H, Jaravel Y and Wooley J C 1980 *Phys. Rev.* B **21** 659
Matsuura M and Kamizato T 1986 *Phys. Rev.* B **33** 8385
McIlroy P W A 1986 *J. Appl. Phys.* **57** 5340
Mendez E E, Agulló-Rueda F and Mong J M 1988 *Phys. Rev. Lett.* **60** 2426
Miller D A B, Chemla D S, Damen T C, Gossard A C, Wiegmann W, Wood T H and Burrus C A 1985 *Phys. Rev.* B **32** 1043
Miller R C, Kleiman D A and Gossard A C 1984 *Phys. Rev.* B **29** 7085
Moyer C 1973 *J. Phys. C: Solid State Phys.* **6** 1461
Pérez-Alvarez R, Rodriguez-Coppola H, Velasco V R and García-Moliner F 1988 *J. Phys. C: Solid State Phys.* **21** 2197
Pötz W and Ferry D K 1985 *Phys. Rev.* B **32** 3863
Trallero-Giner C and López-Gondar J 1986 *Physica* B **138** 287
Viña L, Méndez E, Wang W, Chang L and Esaki L 1987 *J. Phys. C: Solid State Phys.* **20** 2803
Wang W, Méndez E E and Stern F 1984 *Appl. Phys. Lett* **45** 639
Watanabe M O, Yoshida J, Mashita M, Nakanishi T and Hojo A 1985 *J. Appl. Phys.* **57** 5340
West L C and Eglash S J 1985 *Appl. Phys. Lett.* **46** 1156
Wood T H, Burrus C A, Miller D A B, Chemla D S, Damen T C, Gossard A C and Wiegmann W 1984 *Appl. Phys. Lett.* **44** 16
Xu Z Y, Kreismanis V G and Tan C L 1983 *Appl. Phys. Lett* **43** 415
Yamanaka J K, Fukunaga T, Tsukada N, Kobayashi K L I and Ishii M 1986 *Surf. Sci.* **174** 250