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# A method for the calculation of electronic states in a quantum well using the chain model

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**Abstract.** A method for calculating the electronic states in a quantum well (0w) system is presented based on the tight-binding Hamiltonian within a one-band model and in terms of Dyson's equation. The Hamiltonian for the whole system is separated into two parts: one corresponds to an infinitely pure linear chain and the other describes a finite impurity chain confined to the 0w region. The explicit solution to Dyson's equation for the 0w can be obtained via a compact recursion relationship. The formulae have been demonstrated using particular examples. From our numerical evaluation of the energy of the quasi-bound states for the 0w and comparison with the usual effective-mass approximation, it shows that for both models the results are the same. We believe that our treatment may provide great flexibility for dealing with the problem in heterostructures.

## 1. Introduction

Recent progress in semiconductor growth techniques has led to widespread interest in the physics of low-dimensional systems. Quantum wells (Qws), superlattices, double-barrier resonant tunnelling structures have become the objects of extensive investigation (see, e.g., [1, 2]). One of the systems attracting considerable attention is the single well sandwiched between two barriers, in which electrons and holes are confined to a well defined region in space; it leads to the existence of quasi-bound states in the Qw. Various methods and assumptions have been used to evaluate the discrete energy levels associated with the bound states, such as using the effective-mass approximation based on the  $k \times p$  method [3, 4], the self-consistent variational function approach [5, 6], the Green function approach with the tight-binding model [7–9] and so on.

Recently some theoretical considerations have been presented [7, 8] about the density of states of heterostructures within a one-band and a two-band formalism. The calculations are based on a tight-binding Hamiltonian using the transfer-matrix approach via Dyson's equation. This method is exact for a one-dimensional system and seems very appropriate for treating the problem of heterostructures. It was also shown that the application of the effective-mass approximation (EMA) to the calculation of the binding energy is acceptable and valid when compared with the exact results [7, 8].

In this work we present a calculation method for the electronic states in a QW system based on the tight-binding approximation within a one-band model and in terms of



**Figure 1.** Schematic representation of the tight-binding model for the OW system: a finite impurity chain composed of type B atoms embedded in an infinitely pure linear chain composed of type A atoms.

Dyson's equation similar to that presented in [7, 8]. However, we handle the total Hamiltonian of the system in a different way from [7, 8]. First, we consider an infinitely pure chain to serve as our starting point, i.e. an unperturbed system. Then we take into account the contribution of the perturbed potential confined to a finite QW region. This treatment has some advantages. First, we can use the well known Green function for the infinitely pure linear chain. Second, the perturbed potential is concentrated on the narrow QW region; we can then reach an essential simplification by obtaining a set of closed simultaneous equations to determine the one-particle Green function. The explicit solution to these equations can be derived from the recursion relationships. It may make the numerical computation more efficient. It is also clear that our approach may provide great flexibility for dealing with this kind of problem.

We describe the tight-binding Hamiltonian within a one-band model used in our calculation and the basic equations in § 2. The result of numerical calculation and the brief conclusions are given in § 3.

#### 2. The one-band model and the basic equations

Since the one-dimensional model contains the essence of the problem in a QW system, we restrict our work to this case. We assume that the discontinuities in potential for the heterostructure are large enough that the QW can be considered as an isolated QW of finite depth. A schematic representation of the QW geometry used in this work is shown in figure 1. A finite impurity chain composed of type B atoms is embedded in an infinitely pure linear chain composed of type A atoms to form a heterostructure. There is no great loss of generality in assuming that the interaction of the atoms is effective only between nearest neighbours. Let us consider a unit-cell length of the chain. Therefore the tight-binding Hamiltonian for the heterostructure may be expressed in the site representation as

$$H = \sum_{n} \varepsilon_{n} a_{n}^{+} a_{n} + \sum_{m \neq n} \upsilon_{mn} a_{m}^{+} a_{n}$$
<sup>(1)</sup>

where the sum over *m* is limited to nearest neighbours only.  $a_n^+$  and  $a_n$  stand for the *n*th site creation and annihilation operators, respectively. The local site energy  $\varepsilon_n$  is  $\varepsilon_a$  (for a type A atom) or  $\varepsilon_b$  (for a type B atom). The interaction energy  $v_{mn}$  is  $-v_{aa}$  (outside the QW) or  $-v_{bb}$  (inside the QW), or  $-v_{ab}$  at the interface, corresponding to direct-gap semiconductors [9].  $v_{ab}$  is equal to the geometric average of  $v_{aa}$  and  $v_{bb}$ . For definiteness, the site of the type B atom is labelled 1, 2, 3, ..., N. The number of type B atoms is N.

The key mathematical property of the Green function is that it is diagonal in a matrix representation in which the Hamiltonian of the total system is diagonal and that it has

poles at the real values corresponding to the eigenvalues of the system. The density of states for the system is determined by the imaginary part of the Green function for the system.

It is clear that, in order to study the electronic states in the QW, the evaluation of the one-particle Green function for the system becomes the main task. We now separate the whole Hamiltonian into the unperturbed term  $H_a$  and the perturbed term V:

$$H = H_{\rm a} + V \tag{2}$$

where

$$H_{a} = \varepsilon_{a} \sum_{n} a_{n}^{+} a_{n} - v_{aa} \sum_{m \neq n} a_{m}^{+} a_{n}.$$
(3a)

Here the site labels n and m run from minus infinity to plus infinity. Obviously, this Hamiltonian corresponds to a pure linear chain composed of type A atoms. The perturbed Hamiltonian is given by

$$V = -\left(\sum_{n=1}^{N} u_{n,n} a_n^+ a_n + \sum_{n=0}^{N} u_{n+1,n} (a_{n+1}^+ a_n + a_n^+ a_{n+1})\right)$$
(3b)

where

$$u_{n,n} = \epsilon_1 \qquad \text{for } n = 1, 2, 3, \dots, N$$
  

$$u_{n+1,n} = u_{n,n+1} = \epsilon_2 \qquad \text{for } n = 1, 2, 3, \dots, N-1$$
  

$$u_{1,0} = u_{N+1,N} = \epsilon_3$$
  

$$u_{n,n} = u_{n+1,n} = 0 \qquad \text{otherwise} \qquad (3c)$$

and

$$\epsilon_1 = \epsilon_a - \epsilon_b$$
  $\epsilon_2 = v_{bb} - v_{aa}$   $\epsilon_3 = v_{ab} - v_{aa}$  (3d)

This corresponds to the Hamiltonian for a finitely linear chain with interfaces. The oneparticle Green function for the whole system can be determined by the so-called Dyson equation:

$$\boldsymbol{G} = \boldsymbol{G}^0 + \boldsymbol{G}^0 \boldsymbol{V} \boldsymbol{G} \tag{4}$$

where  $G^0$  denotes the one-particle Green function for the regularly linear chain. Introducing the transfer matrix defined by [7]

$$T(\omega) = G_{n+m+1,n}^0 / G_{n+m,n}^0$$
 for  $m > 0$ 

and

$$T(\omega) = G_{n+m-1,n}^0 / G_{n+m,n}^0 \qquad \text{for } m < 0 \tag{5}$$

Thus the matrix elements for  $G^0$  are then connected with each other via the transfer matrix T as

$$G_{n+m,n}^{0} = T^{|m|} G_{nn}^{0} \tag{6}$$

and the particular expression for the *T*-function is [7]

$$T(\omega) = (1/2\nu_{aa}) \left[ -(\omega - \varepsilon_{a}) + \text{sgn}(\omega - \varepsilon_{a})\sqrt{(\omega - \varepsilon_{a})^{2} - 4\nu_{aa}^{2}} \right]$$
(7)

where sgn(x) means taking the sign of the value x. The T-function is complex in the interval

$$-2v_{aa} < \omega - \varepsilon_a < 2v_{aa} \tag{8}$$

which corresponds to the energy band of the regular chain. The diagonal elements for  $G^0$  in the site representation are well known [10], i.e.

$$G_{nn}^{0} = g_{0} = i \operatorname{sgn}(\omega - \varepsilon_{a}) / \sqrt{4v_{aa}^{2} - (\omega - \varepsilon_{a})^{2}}.$$
(9)

We are now in a position to calculate the Green function G for the whole system. Dyson's equation (4) can be expresed in terms of the matrix elements in the site representation as

$$G_{ij} = G_{ij}^0 + \Delta G_{ij} = G_{ij}^0 + \sum_{p.m} G_{ip}^0 V_{pm} G_{mj}$$
(10)

where the site labels *i* and *j* run over the whole system.

Using the particular expressions (3b) and (3c) for V, the equation (10) becomes a set of linearly coupled equations:

$$G_{ij}^{0} = T^{|i-j|} g_{0} = \sum_{p=0}^{N+1} (\delta_{ip} + \Phi_{ip}) G_{pj} \qquad \text{for } -\infty < i, j < +\infty$$
(11)

where

$$\begin{split} \Phi_{p,p} &= 1 + a_p \qquad p = 0, 1, 2, \dots, N + 1 \\ \Phi_{i,p} &= b_p T^{i-p} \qquad i > p, p = 0, 1, 2, \dots, N + 1 \\ &i = p + 1, p + 2, \dots, N + 1 \\ \Phi_{i,p} &= c_p T^{p-i} \qquad i < p, i = 0, 1, 2, \dots, N + 1 \\ &p = i + 1, i + 2, \dots, N + 1 \\ \Phi_{i,p} &= 0 \qquad \text{otherwise} \end{split}$$
(12a)

and

$$a_{i} = (u_{i-1,i}T + u_{i,i} + u_{i+1,i}T)g_{0}$$
  

$$b_{i} = (u_{i-1,i}T + u_{i,i} + u_{i+1,i}T^{-1})g_{0}$$
  

$$c_{i} = (u_{i-1,i}T^{-1} + u_{i,i} + u_{i+1,i}T)g_{0}.$$
(12b)

Note that the matrix  $\Phi$  does not depend on the subscript *j*.

To obtain the one-particle Green function for the whole system, we need to solve the inhomogeneously coupled equations (11). We now consider the ow region and the interface. Consequently, we take into account only the sites labelled from 0 to N + 1. The rank of the set of equations becomes N + 2. We can write Dyson's equations in an explicit version as follows:

The superscript T denotes the transposition operation. Because the coefficients appearing in the equation (13) exhibit obvious regularity, by using the standard operation such as Laplace's development of the determinant [11], through many time-consuming and cumbersome operations, we can finally derive a solution to equations (13) as follows (see Appendix for details):

$$G_{ii}(\omega) = B_{ii}(\omega)/D_{N+2}(\omega)$$
 for  $j = 0, 1, 2, ..., N+1$ . (14)

 $D_{N+2}(\omega)$  can be evaluated via the following recursion relationships:

$$D_{k} = \alpha_{N+2-k} D_{k-1} + (-1)^{k-1} \xi_{N+2-k} F_{k-1}$$

$$D_{0} = 1 \qquad D_{1} = \alpha_{N+1} \qquad D_{2} = \alpha_{N} \alpha_{N+1} - \xi_{N} \bar{\beta}_{N+1}.$$
(15)

 $F_{k-1}(\{\alpha_i\}, \{\beta_i\}, \{\gamma_i\})$  satisfies the other recursion relation

$$F_{k} = \beta_{N+2-k} F_{k-1} - \alpha_{N+2-k} \gamma_{N+3-k} F_{k-2}$$

$$F_{0} = 1 \qquad F_{1} = \overline{\beta}_{N+1} \qquad F_{2} = \beta_{N} \overline{\beta}_{N+1} - \alpha_{N} \gamma_{N+1}.$$
(16)

Here the coefficients are the combinations of the  $\{a_i\}, \{b_i\}$  and  $\{c_i\}$  as

$$\begin{aligned} \alpha_{i} &= 1 + a_{i} - b_{i} & i = 0, 1, 2, \dots, N + 1 \\ \beta_{i} &= -[(1 + a_{i})/T + (1 + a_{i} - b_{i} - c_{i})T] & i = 1, 2, 3, \dots, N \\ \bar{\beta}_{N+1} &= -[(1 + a_{N+1})/T - c_{N+1}T] & (17) \\ \gamma_{i} &= 1 + a_{i} - c_{i} & i = 2, 3, 4, \dots, N + 1 \\ \xi_{i} &= b_{i}T^{|N+1-i|} & i = 0, 1, 2, 3, \dots, N \\ \alpha_{i} &= \gamma_{i} = 1 & \beta_{i} = \xi_{i} = 0 & \text{otherwise.} \end{aligned}$$

For the numerator  $B_{ij}(\omega)$  of the solution, it can be estimated by using the similar recursion relations (15) and (16) with some different coefficients

$$\begin{aligned}
\alpha_j &= 0 & \beta_j = g_0 (T - 1/T) \\
\gamma_j &= 0 & \xi_j = g_0 T^{\langle N+1-j \rangle} & \text{for } G_{jj}.
\end{aligned}$$
(18)

The other coefficients remain unchanged. The zeros of  $G_m^{-1}$  give the energy levels of the

quasi-bound states inside the QW, as are determined by  $D_{N+2}(\omega) = 0$ . The density of the states is then determined by

$$\rho(\omega) = -\frac{1}{\pi} \operatorname{Im}\left(\sum_{n} G_{nn}(\omega)\right).$$
(19)

To demonstrate that the recursion relations are correct, we apply them to the simplest case. A gw is composed of only two nearest-neighbour atoms and only the diagonal interaction between the two impurity atoms is effective. We label the sites of the impurity atoms 1 and 2, the interaction potential is taken as  $v_{aa} = v_{bb} = v_{ab}$  and  $u_{1,1} = u_{2,2} = \varepsilon_a - \varepsilon_b$ . Corresponding to this particular case, we have N = 2 and

$$a_{1} = b_{1} = c_{1} = u_{1,1}g_{0} \qquad a_{2} = b_{2} = c_{2} = u_{2,2}g_{0}$$

$$a_{i} = b_{i} = c_{i} = 0 \qquad \text{otherwise.}$$
(20)

Substituting these parameters into equation (17), one obtains

$$\begin{aligned}
\alpha_i &= 1 \qquad \gamma_i = 1 \qquad \text{for any } i \\
\beta_1 &= -[(1 + u_{1,1}g_0)/T + (1 - u_{1,1}g_0)T] \\
\beta_2 &= -[(1 + u_{2,2}g_0)/T + (1 - u_{2,2}g_0)T] \\
\bar{\beta}_3 &= -1/T \qquad \beta_i = 0 \qquad \text{for } i \ge 4.
\end{aligned}$$
(21)

By using the recursion relationships (15) and (16), one obtains

$$D_4(\omega) = D_1 - b_2 T F_1 + b_1 T^2 F_2 = \alpha_3 - b_2 T \bar{\beta}_3 + b_1 T^2 (\beta_2 \bar{\beta}_3 - \alpha_2 \gamma_3)$$
  
=  $(1 + u_{1,1} g_0) (1 + u_{2,2} g_0) - u_{1,1} u_{2,2} g_0^2 T^2.$  (22)

This expression agrees completely with that given in [10].

#### 3. Numerical calculations and conclusions

To see whether our particular approach can be used to treat the problem of heterostructures, we need to perform numerical calculations for some specific examples. We choose the set of parameters given in [7] for GaAs-(Ga, Al)As, i.e.  $E_a = 0.22$  and 0.14 eV,  $E_b = 0$ ; only the difference  $E_a - E_b$  is involved in our formulae. We take  $v_{aa} = v_{bb} = 7.0 \text{ eV}$ . The width of the QW is Na, where N is the number of the type B atoms composing the QW, and a is the cell length of the chain. In table 1 we present the calculated energy of the quasi-bound states inside the QW for different widths of the well.

To compare our calculated result with that obtained by the usual EMA, we also perform an elementary quantum mechanical calculation. We need to solve the following transcendental equation to determine the discrete energy levels in a rectangular QW of finite depth equal to  $V_0 = |E_a - E_b|$  and of width Na [12]:

$$N\sqrt{E/|v_{\rm aa}|} = n\pi - 2\sin^{-1}\sqrt{E/V_0}$$

where *n* is taken to be an integral number (n = 1, 2, 3, ...). Here we consider that the effective mass is related to  $|v_{aa}|$  by [9]

$$m^* = \hbar^2/2|v_{\rm aa}|a^2.$$

For simplicity we assume that for both types of atom the effective masses are the same.

N	$V_0 = 0.22 (eV)$ present work	$V_0 = 0.22 (eV)$ EMA	$V_0 = 0.14 (eV)$ present work	$V_0 = 0.14 (eV)$ EMA		
10	0.13140	0.13174	0.09675	0.09689		
40	0.02600 0.10050 0.20372	0.02603 0.10068 0.20402	0.02319 0.08708	0.02320 0.08719		
80	0.00830 0.03300 0.07360 0.12800 0.19260	0.00828 0.03295 0.07342 0.12826 0.19297	0.00778 0.03083 0.06801 0.11553	0.00777 0.03080 0.06797 0.11569		

Table 1. Energy of quasi-bound states in the Qws.

It is interesting to note that the result calculated from our model, which is exact for a one-dimensional system and beyond the EMA, is the same as that obtained by the EMA. It is evidence that the EMA is very suitable for treating the problem of heterostructures, as indicated in [7].

Although we use the same tight-binding model for the heterostructures in this paper as that presented in [7, 8], our calculated scheme is different from that in [7, 8]. The unperturbed system and the perturbed effect are handled separately. We can use the well known one-particle Green function for the infinitely regular chain to estimate the Green function for the whole system. To investigate the electronic states in the Qw, it involves solving only the simultaneously linear equations with N + 2 rank. The explicit solution can be expressed by the compact recursion relationships. Therefore, it may provide a more efficient numerical computation. For asymmetric barriers, e.g. for the various potential profiles under the application of a DC electric field, and for a Qw made by amorphous materials, our approach provides a uniform treatment and may be shown to be more powerful, convenient and rapid. The advanced results are presented in a forthcoming paper.

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### Appendix

We now briefly present some evaluations for the relevant determinant appearing in the text. To simplify the description of the calculated process, we introduce the following symbols to represent the corresponding operation procedure.

(i) Operate an  $N \times N$  determinant by subtracting (adding) c times the (i - 1)st row (column) from the *i*th row (column), and then subtract c times the (i - 2)nd row (column) from the (i - 1)st row (column), etc,

$$i$$
th  $\mp c(i-1)$ st  $\rightarrow i$ th row (column)  $i = 2, 3, 4, \dots, N.$ 

(ii) Operate on an  $N \times N$  determinant A by performing the so-called Laplace development according to its *j*th column (row) [11], i.e.

$$A = \sum_{j=1}^{N} a_{1j} A_{1j}$$
 or  $A = \sum_{j=1}^{N} a_{j1} A_{j1}$ .

This is the sum of the products of the elements of the *j*th column (row) of A and their respective cofactors. We symbolise this as

Dev A to *j*th column (row).

To solve Dyson's equations for the QW system, we meet the following determinant:

$1 + a_0$	$c_1 T$	$c_{2}T^{2}$	$c_{3}T^{3}$	•••	$c_{N-1}T^{N-1}$	$c_N T^N$	$c_{N+1}T^{N+1}$	
$b_0 T$	$1 + a_1$	$c_2T$	$c_3 T^2$	•••	$c_{N-1}T^{N-2}$	$c_N T^{N-1}$	$c_{N+1}T^N$	
$b_0 T^2$	$b_1T$	$1 + a_2$	$c_3T$		$c_{N-1}T^{N-3}$	$c_N T^{N-2}$	$c_{N+1}T^{N-1}$	
•••	•••	•••		•••	•••		••••	(A1)
•••	•••		•••		•••	•••		(/
$b_0 T^{N-1}$	$b_1 T^{N-2}$	$b_2 T^{N-3}$	$b_3 T^{N-4}$		$1 + a_{N-1}$	$c_N T$	$c_{N+1}T^2$	
$b_0 T^N$	$b_1 T^{N-1}$	$b_2 T^{N-2}$	$b_3 T^{N-3}$		$b_{N-1}T$	$1 + a_{N}$	$c_{N+1}T$	
$b_0 T^{N+1}$	$b_1 T^N$	$b_2 T^{N-1}$	$b_3 T^{N-2}$		$b_{N-1}T^2$	$b_N T$	$1 + a_{N+1}$	

We calculate this by the following procedure.

(i) ith  $-(T^{-1}) \times (i + 1)$ st  $\rightarrow i$ th row, for i = 1, 2, 3, 4, ..., N + 1. All the elements below the diagonal line become zero with the exception of the last row. For the modified  $D_{N+2}$ , we continue to operate.

(ii) ith  $-(T) \times (i + 1)$ st  $\rightarrow i$ th row for i = 1, 2, 3, ..., N; the last two rows remain unchanged. Thus  $D_{N+2}$  has the upper tridiagonal form in which the element is zero apart from the diagonal and two lines of elements immediately to the upper side of it. Of course, the elements of the last row still exist, i.e.

	$\alpha_0$	$\beta_1$	$\gamma_2$	0	0	•••	•••	0	0	
	0	$\alpha_1$	$\beta_2$	γ3	0			0	0	н 1997 - Эл
	0	0	α2	$\beta_3$	$\gamma_4$			0	0	
$D_{N+2}(\{\alpha_i\},\{\beta_i\},\{\gamma_i\},\{\xi_i\}) =$	•••		•••	•••	•••		••••			(A2)
			•••	•••	•••	•••	•••	•••		
	0	0	0	0	0	•••		$\alpha_N$	$\bar{\beta}_{N+1}$	
	$\xi_0$	ξ1	ξ2	ξ3	ξ4	•••		$\xi_N$	$\alpha_{N+1}$	

where the relationship between  $\{\alpha_i\}, \{\beta_i\}, \{\gamma_i\}, \{\xi_i\}$  and  $\{a_i\}, \{b_i\}, \{c_i\}$  are given by equation (17) in the text. We now perform the following.

(iii) Dev the modified  $D_{N+2}$  to the first column. We have

$$D_{N+2} = \alpha_0 D_{N+1} + (-1)^{N+3} \xi_0 F_{N+1}.$$
 (A3)

The general recursion relation can be written as

$$D_{k} = \alpha_{N+2-k} D_{k-1} + (-1)^{k+1} \xi_{N+2-k} F_{k-1}$$
(A4a)

and

$$D_0 = 1$$
  $D_1 = \alpha_{N+1}$   $D_2 = \alpha_N \alpha_{N+1} - \xi_N \bar{\beta}_{N+1}.$  (A4b)

The second determinant  $F_{n+1}(\{\alpha_i\}, \{\beta_i\}, \{\gamma_i\})$  is defined by

It is in the exact tridiagonal form. We can readily derive the recursion relation to be satisfied by  $F_{N+1}$ :

$$F_{N+1} = \beta_1 F_N - \alpha_1 \gamma_2 F_{N-1}.$$
 (A6)

The general term can be expressed as

$$F_{k} = \beta_{N+2-k} F_{k-1} - \alpha_{N+2-k} \gamma_{N+3-k} F_{k-2}$$
(A7a)

and

$$F_0 = 1$$
  $F_1 = \bar{\beta}_{N+1}$   $F_2 = \beta_N \bar{\beta}_{N+1} - \alpha_N \gamma_{N+1}.$  (A7b)

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