Calculation of the band structure of semiconductor quantum wells using scattering matrices

1996 J. Phys.: Condens. Matter 8 10347

(http://iopscience.iop.org/0953-8984/8/49/024)

J. Phys.: Condens. Matter **8** (1996) 10347–10352. Printed in the UK

Calculation of the band structure of semiconductor quantum wells using scattering matrices

Wei-Dong Sheng

CCAST (World Laboratory) PO Box 8730, Beijing, 100080, and National Laboratory for Superlattices and Microstructures, Institute of Semiconductors, Chinese Academy of Sciences, PO Box 912, Beijing 100083, People's Republic of China

Received 10 June 1996, in final form 19 August 1996

Abstract. The transfer-matrix method widely used in the calculation of the band structure of semiconductor quantum wells is found to have limitations due to its intrinsic numerical instability. It is pointed out that the numerical instability arises from free-propagating transfer matrices. A new scattering-matrix method is developed for the multiple-band Kane model within the envelope-function approximation. Compared with the transfer-matrix method, the proposed algorithm is found to be more efficient and stable. A four-band Kane model is used to check the validity of the method and the results are found to be in good agreement with earlier calculations.

In order to understand the transport properties and features exhibited in the optical spectrum of semiconductor quantum wells and superlattices, it is essential to calculate the pertinent electronic band structure. Besides the tight-binding approach [1], the envelope-function approximation (EFA) [2] is also widely used in the calculation of the band structure of quantum wells and superlattices. Within EFA formalism, the band structure is calculated by adopting the Luttinger–Kohn model [3] and a set of coupled second-order differential equations for the envelope functions are solved in the numerical calculation. There have been many methods proposed for solving the simultaneous equations, e.g., the variational approach [4], transfer-matrix methods [2, 5, 6], and the finite-difference method [7].

Although the transfer-matrix method has been extensively used in the context of the Kronig–Penney model and multiple-band Kane model, we will show that the algorithm is not stable in the numerical calculation and that it cannot be adapted to quantum wells of arbitrary dimensions and layer interleaving. The intrinsic numerical instability of the transfer-matrix method has also been established in other areas [8, 9]. The shortcomings of the transfer-matrix method can be completely overcome by using the scattering-matrix technique [9]. In this paper, we propose a scattering-matrix approach to the calculation of the band structure of semiconductor quantum wells on the basis of the multiple-band Kane model.

Let us consider the case of multiple quantum wells and set the z-axis to be perpendicular to the layers. Within the context of the multiple-band Kane model [11], the envelope functions $\Psi(r)$ in each layer satisfy the effective-mass equation [10]

$$\begin{aligned} &H\Psi(r) = E\Psi(r) \\ &H = \hat{k}_z A \hat{k}_z + (\hat{k}_z B + B\hat{k}_z)/2 + C + V \end{aligned} \tag{1}$$

where V is the potential arising from the band offsets and is assumed to be constant in each layer. The envelope function can be expanded as a linear combination of the corresponding

0953-8984/96/4910347+06$19.50

bulk solution for a given E, k_x, and k_y. For some simple cases, e.g. the widely used 4×4 Kane model neglecting the conduction and spin–orbit bands, solutions for the effective-mass equation in the bulk can be given analytically [2]. Here, we apply a simple algorithm to solve the bulk problem because it is very difficult to provide analytical solutions if the Hamiltonian is of larger dimensions.

For a given E, k_x, and k_y, the solution for the effective-mass equation in the bulk can be written as $\Psi = \mathrm{e}^{\mathrm{i}kz}\mathbf{F}$, where $\mathbf{F}$ is a combination of Luttinger–Kohn or Kane wave functions and satisfies the relation

$$[Ak^2 + Bk + (C + V - E)]\mathbf{F} = 0. \tag{2}$$

Defining $\mathbf{F}' = k\mathbf{F}$, the equation can be rewritten as

$$\begin{bmatrix} \mathbf{0} & \mathbf{I} \\ -A^{-1}(C + V - E) & -A^{-1}B \end{bmatrix} \begin{bmatrix} \mathbf{F} \\ \mathbf{F}' \end{bmatrix} = k \begin{bmatrix} \mathbf{F} \\ \mathbf{F}' \end{bmatrix}. \tag{3}$$

Solving the equation, we can obtain $2N$ eigenvalues $\pm k_n$ and eigenvectors $\mathbf{F}_n^{\pm}$, where N is the number of the bands considered in the model. The wave function can be expanded as

$$\Psi(z) = \sum_{n=1}^{N} (c_n^+ \mathrm{e}^{\mathrm{i}k_n z}\mathbf{F}_n^+ + c_n^- \mathrm{e}^{-\mathrm{i}k_n z}\mathbf{F}_n^-). \tag{4}$$

Hence it can be described by a vector $\mathbf{C} = [\mathbf{C}^+, \mathbf{C}^-]^{\mathrm{T}}$, where $\mathbf{C}^{\pm}$ are N-dimensional column vectors with elements $c_n^{\pm}$. Using the boundary conditions given in references [10] and [12], the following relation can be obtained at the interface between layer i and layer j:

$$\begin{aligned} &\mathbf{M}_i\mathbf{C}_i = \mathbf{M}_j\mathbf{C}_j \\ &\mathbf{M}_{i,j} = \begin{bmatrix} \mathbf{F}_{i,j}^+ & \mathbf{F}_{i,j}^- \\ \mathbf{J}_{i,j}^+ & \mathbf{J}_{i,j}^- \end{bmatrix} \end{aligned} \tag{5}$$

where $\mathbf{F}^{\pm}$ and $\mathbf{J}^{\pm}$ are N-dimensional matrices with columns $\mathbf{F}_n^{\pm}$ and $\mathbf{J}_n^{\pm} = (\pm Ak_n + B/2)\mathbf{F}_n^{\pm}$, respectively.

A free-propagating transfer matrix $\mathbf{P}$ connecting two ends of a layer of width d is given by

$$\mathbf{P} = \begin{bmatrix} \mathbf{P}^- & \mathbf{0} \\ \mathbf{0} & \mathbf{P}^+ \end{bmatrix} \tag{6}$$

where $\mathbf{P}^{\pm}$ are diagonal matrices with elements $\mathrm{e}^{\pm \mathrm{i}k_n d}$. Supposing that the total number of layers is N_L, the overall transfer matrix is then constructed by the multiplication of the interface and free-propagating transfer matrices [12]:

$$\mathbf{T} = \mathbf{T}_{1,2}\mathbf{P}_2 \cdots \mathbf{P}_{N_L-1}\mathbf{T}_{N_L-1,N_L} \tag{7}$$

where $\mathbf{T}_{n-1,n}$ is the transfer matrix associated with the interface between layer $n-1$ and layer n and is given by $\mathbf{T}_{n-1,n} = \mathbf{M}_{n-1}^{-1}\mathbf{M}_n$ from equation (5).

If the overall transfer matrix is written in the block form

$$\mathbf{T} = \begin{bmatrix} \mathbf{T}_{11} & \mathbf{T}_{12} \\ \mathbf{T}_{21} & \mathbf{T}_{22} \end{bmatrix} \tag{8}$$

then the band structure can be obtained by finding the zeros of the determinant of $\mathbf{T}_{11}$. But it is found that the transfer-matrix method cannot provide all of the energy levels of the quantum wells especially when the in-plane wavenumber k_x or k_y is not close to the Γ point. Figure 1 shows the scanning result obtained from the transfer-matrix method for a GaAs/$Al_{0.25}Ga_{0.75}$As single quantum well (100 Å) and multiple quantum wells

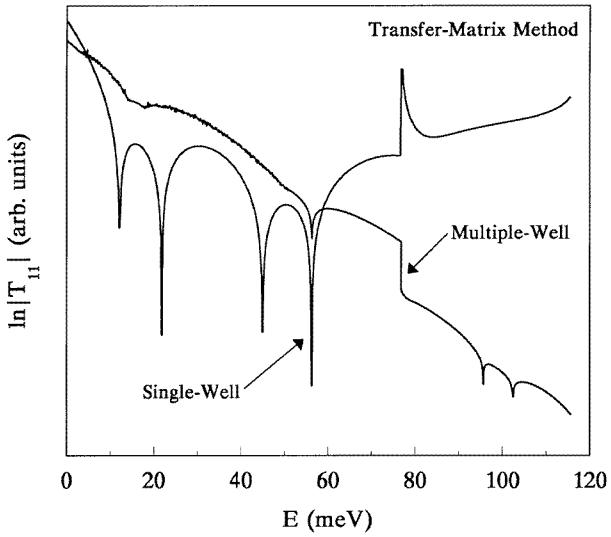

Figure 1. The result from the transfer-matrix method for a GaAs/$Al_{0.25}Ga_{0.75}As$ single quantum well (100 Å) and multiple quantum wells (100 Å/300 Å) for $k_x = 0.02$ Å^{-1} and $k_y = 0.01$ Å^{-1} obtained using the four-band Kane model.

(100 Å/300 Å) for $k_x = 0.02$ Å^{-1} and $k_y = 0.01$ Å^{-1} using the four-band Kane model [2]. There should be six energy levels in this kind of structure under the valence band offset 120 meV, while the results cannot give all of the levels for all possible single- or multiple-quantum-well structures. The same problem also arises in another transfer-matrix method [5] which is slightly different from one described above. We would like to note that the transfer-matrix method is also found not to be stable in the calculation of the conductance of one-dimensional disordered systems [9].

The numerical instability of the transfer-matrix method arises from $\mathbf{P}^-$. In a layer where V is larger than E, some of $\pm k_n$s would not be real and the corresponding P_{nn}^- would become much larger, especially for layers of large width. Therefore, the transfer-matrix method cannot apply to the case of the structure containing barriers of large dimensions.

The numerical instability of the transfer-matrix method can be completely removed by using the scattering-matrix technique. Within the scattering-matrix formalism, the wave functions of the two adjacent layers i and j are related by a scattering matrix:

$$\begin{bmatrix} \mathbf{C}_i^- \\ \mathbf{C}_j^+ \end{bmatrix} = \mathbf{S}_{i,j} \begin{bmatrix} \mathbf{C}_i^+ \\ \mathbf{C}_j^- \end{bmatrix}$$

$$\mathbf{S}_{i,j} = \begin{bmatrix} \mathbf{F}_i^- & -\mathbf{F}_j^+ \\ \mathbf{J}_i^- & -\mathbf{J}_j^+ \end{bmatrix}^{-1} \begin{bmatrix} \mathbf{F}_i^+ & -\mathbf{F}_j^- \\ \mathbf{J}_i^+ & -\mathbf{J}_j^- \end{bmatrix}. \tag{9}$$

The scattering matrix for free propagation between two ends of a layer of width d is given by

$$\mathbf{S}^{free} = \begin{bmatrix} \mathbf{0} & \mathbf{P}^+ \\ \mathbf{P}^+ & \mathbf{0} \end{bmatrix}. \tag{10}$$

The overall scattering matrix for the structure containing a certain number of wells and barriers can be obtained by decomposing it into interface parts and free-propagating parts

using a composition law [13]. Considering two scattering matrices defined by

$$\mathbf{S}_1 = \begin{bmatrix} \mathbf{r}_1 & \mathbf{t}'_1 \\ \mathbf{t}_1 & \mathbf{r}'_1 \end{bmatrix} \qquad \text{and} \qquad \mathbf{S}_2 = \begin{bmatrix} \mathbf{r}_2 & \mathbf{t}'_2 \\ \mathbf{t}_2 & \mathbf{r}'_2 \end{bmatrix} \tag{11}$$

where $\mathbf{t}, \mathbf{t}'$, and $\mathbf{r}, \mathbf{r}'$ are the transmission and reflection probabilities for fluxes incident from the left and right respectively, the composed scattering matrix $\mathbf{S}_{12}$ constructed from $\mathbf{S}_1$ and $\mathbf{S}_2$ can be calculated as

$$\begin{aligned} \mathbf{t}_{12} &= \mathbf{t}_2(\mathbf{I} - \mathbf{r}'_1\mathbf{r}_2)^{-1}\mathbf{t}_1 \\ \mathbf{t}'_{12} &= \mathbf{t}'_1(\mathbf{I} - \mathbf{r}_2\mathbf{r}'_1)^{-1}\mathbf{t}'_2 \\ \mathbf{r}_{12} &= \mathbf{r}_1 + \mathbf{t}'_1\mathbf{r}_2(\mathbf{I} - \mathbf{r}'_1\mathbf{r}_2)^{-1}\mathbf{t}_1 \\ \mathbf{r}'_{12} &= \mathbf{r}'_2 + \mathbf{t}_2\mathbf{r}'_1(\mathbf{I} - \mathbf{r}_2\mathbf{r}'_1)^{-1}\mathbf{t}'_2. \end{aligned} \tag{12}$$

For convenience, the above procedures are denoted by an operator $\otimes$, i.e., $\mathbf{S}_{12} = \mathbf{S}_1 \otimes \mathbf{S}_2$.

The overall scattering matrix is then expressed as

$$\mathbf{S} = \mathbf{S}_{1,2} \otimes \mathbf{S}_2^{free} \otimes \cdots \otimes \mathbf{S}_{N_L-1}^{free} \otimes \mathbf{S}_{N_L-1,N_L}. \tag{13}$$

If the overall transfer matrix is written in a block form similar to equation (8), we have the relation $\mathbf{S}_{21} = -\mathbf{T}_{11}^{-1}$. Hence the band structure can be obtained by finding the maximum value of the determinant of $\mathbf{S}_{21}$.

The scattering-matrix approach to calculations of the band structure does not limit itself to the case of rectangular quantum wells. More general well potentials can be approximated by a series of constant steps and the number of the steps should be sufficiently large to provide the desired convergence in the result. In this piecewise approximation scheme, the coefficients c_n and k_n in equation (4) would be position dependent.

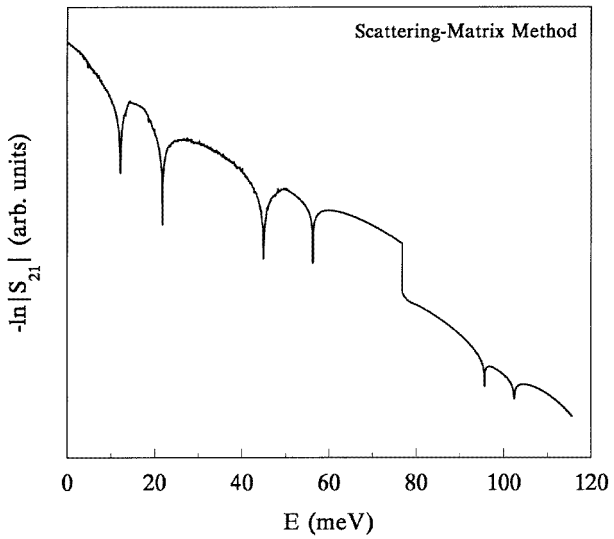

Figure 2. The result obtained from the scattering-matrix method for GaAs/$Al_{0.25}Ga_{0.75}$As multiple quantum wells. The parameters are the same as those in figure 1.

In figure 2, we provide the scanning result obtained from the scattering-matrix method for GaAs/$Al_{0.25}Ga_{0.75}$As multiple quantum wells. The parameters are the same to those adopted in figure 1. From the result, we find that all six energy levels are clearly shown. In

the numerical calculation, we also find that the scattering-matrix algorithm is not sensitive to the dimensions of the barriers.

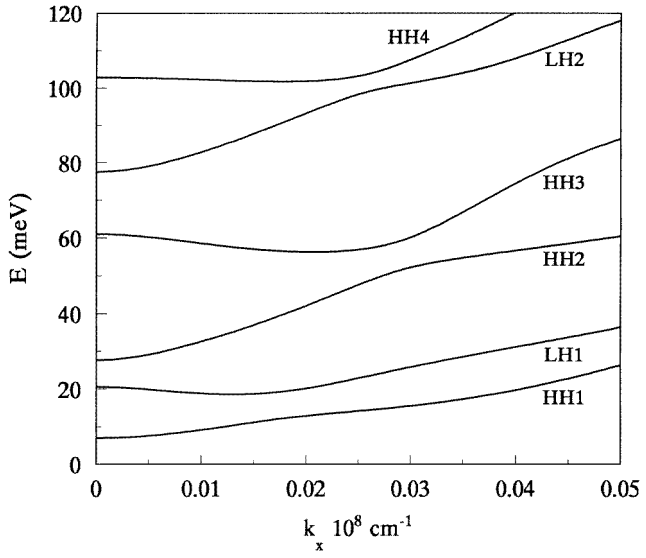

Figure 3. The valence band structure of $GaAs/Al_{0.25}Ga_{0.75}As$ multiple quantum wells (100 Å/300 Å) for $k_y = 0$ calculated by the scattering-matrix method.

In order to check the validity of the scattering-matrix method, we calculate the valence band structure of $GaAs/Al_{0.25}Ga_{0.75}As$ multiple quantum wells (100 Å/300 Å) and the results are given in figure 3. Similar structures have been calculated by many authors and the comparison between our results and those in the literature shows that the results from the scattering-matrix method are in good agreement with earlier calculations.

In summary, we have found that the transfer-matrix method widely used in the calculation of the band structure of semiconductor quantum wells has limitations due to its intrinsic numerical instability. We have pointed out that the numerical instability arises from free-propagating transfer matrices. We have proposed a new scattering-matrix method for the multiple-band Kane model within the envelope-function approximation. Compared with the transfer-matrix method, the proposed algorithm has been found to be more efficient and stable. We have used the four-band Kane model to check the validity of the method and found that the results are in good agreement with earlier calculations.

Acknowledgment

This work was supported by the Chinese National Science Foundation.

References

[1] Schulman J N and McGill T C 1977 *Phys. Rev. Lett.* **39** 1680
[2] Wessel R and Altarelli M 1989 *Phys. Rev.* B **39** 12 801
[3] Luttinger J M and Kohn W 1955 *Phys. Rev.* **97** 869
[4] Broido D A and Sham L J 1985 *Phys. Rev.* B **31** 888
[5] Ram-Mohan L R, Yoo K H and Aggarwal R L 1988 *Phys. Rev.* B **38** 6151

[6] Harwit A, Harris J S and Kapitulnik A 1986 *J. Appl. Phys.* **60** 3211
[7] Ogawa M and Miyoshi T 1995 *Japan. J. Appl. Phys.* **34** 3043
[8] Baranger H U, DiVincenzo D P, Jalabert R A and Stone A D 1991 *Phys. Rev.* B **44** 10 637
[9] Bandyopadhyay S and Cahay M 1991 *Computational Electronics: Semiconductor Transport and Device Simulation* ed K Hess (Boston, MA: Kluwer Academic) p 223
[10] Bastard G 1988 *Wave Mechanics Applied to Semiconductor Heterostructures* (Paris: Editions de Physique)
[11] Kane E O 1966 *Semiconductors and Semimetals* vol 1, ed R K Willardson and A C Beer (New York: Academic) p 75
[12] Chao C Yi-Ping and Chuang S L 1991 *Phys. Rev.* B **43** 3027
[13] Anderson P W 1981 *Phys. Rev.* B **23** 4828