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# A continued-fraction approach for the numerical determination of one-dimensional band structures

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**Abstract.** A discretisation scheme is used to obtain a numerical solution of periodic one-dimensional Schrödinger equations. Using a continued fraction leads to a very simple algorithm for the computation of energy band edges and dispersion laws inside the allowed bands.

## 1. Introduction

The elucidation of many aspects of the behaviour of solid materials owes much to the early discovery of the energy band systems associated with three-dimensional periodic potentials. Many of the ideas developed for understanding the quantum mechanics of electrons in lattices originate from the consideration of some exactly soluble one-dimensional problems (Kronig and Penney 1931, Scarf 1958). Of course, one-dimensional examples are far from giving a complete account of the variety of situations arising when real band structure calculations are carried out. It is not surprising, in that respect, that one-dimensional periodic models were disregarded as soon as efficient methods for treating three-dimensional cases were developed (see e.g. Callaway 1976). However, a Kronig-Penney model has recently been brought back to light with the achievement of periodically layer-structured semiconductors by means of the technique of molecular beam epitaxy (Dingle 1976, Esaki 1978). The Kronig-Penney model is generally applied to such systems, though the real effective potential felt by the conduction electrons in the one-dimensional superlattice is sometimes not very accurately represented by a square-top function. On the other hand, the rapid development of graded mixed semiconductors allows for the preparation of samples presenting a wide range of effective potentials, so that many different kinds of one-dimensional periodic structures could be prepared. The theoretical treatment of such systems obviously needs the consideration of a one-dimensional Schrödinger equation corresponding to a general periodic potential.

The numerical solution of one-dimensional Schrödinger equations is now customary. Different approaches are competing. The best known are based on the finite-differences method (Hajj *et al* 1974) or the finite-elements method (Golub *et al* 1975, Friedman *et al* 1978). Recently Raptis and Allison (1978) reported a new multi-step method well suited for bound states. In contrast with the radial potential, the one-dimensional periodic Schrödinger equation has not received any particular interest. The aim of this paper is to present a very simple way of solving the band structure

problem for any one-dimensional periodic potential. The proposed method does not require the use of a powerful computer.

In essence, the calculation is similar to the simple ('pocket calculator') technique described by Killingbeck (1977a, b), designed to determine the energy eigenvalues corresponding to bound states. The starting scheme is the well-known difference equation

$$(\psi(x+h) - 2\psi(x) + \psi(x-h))/h^2 = (v(x) - \epsilon)\psi(x), \quad (1.1)$$

which models the Schrödinger equation

$$d^2\psi(x)/dx^2 = (v(x) - \epsilon)\psi(x) \quad (1.2)$$

with a truncation error proportional to  $h^2$ . As pointed out by Gautschi (1967), a close relation exists between three-term recursions and continued fractions. The continued fraction generated by equation (1.1) will be extensively used to obtain, in a very simple way, a very good approximation to the band structure.

The formalism is described in § 2, where the secular equation is derived. In an original way, the alternation of forbidden and allowed energy bands is simply related to the variations of a polynomial function of the energy. An analytical expression of the dispersion relation is also obtained. This relation exhibits all the symmetry properties of the continuous Schrödinger equation. This seems to indicate that the discretising technique used in the present approach is particularly well suited for solving the problem considered in this paper.

## 2. Properties and solution of the discrete periodic equation

The question of describing the energy spectrum corresponding to a periodical potential is twofold:

(i) at which values of the energy are the allowed band limits located?

(ii) inside an energy band, what is the dispersion relation between the energy and a Bloch wavevector?

In both cases, the continued fraction approach will provide a very general and efficient answer. Let us suppose that the interval  $(x_0, x_{n+1})$  is a period of the potential function  $v(x)$ . Inside this interval, let us define the grid  $x_1, x_2, \dots, x_n$  which divides the period into  $n+1$  equal parts of length

$$h = (x_{n+1} - x_0)/(n+1). \quad (2.1)$$

Due to the periodicity of the potential, the solution  $\psi(x)$  of the discretised Schrödinger equation verifies the Bloch theorem, i.e. can be written as

$$\psi(x) = u_k(x) e^{ikx}, \quad (2.2)$$

where the function  $u_k(x)$  has the same periodicity as the potential and, for any allowed energy values,  $k$  is a real wavenumber. Then equation (1.1) can be rewritten as

$$e^{-ikh} \frac{u_k(x_{p-1})}{u_k(x_p)} = b_p(\epsilon) - \frac{1}{e^{-ikh} u_k(x_p)/u_k(x_{p+1})}, \quad (2.3)$$

where

$$b_p(\epsilon) = 2 + h^2(v(x_p) - \epsilon). \quad (2.4)$$

If we introduce the notation

$$R_p = e^{-ikh} u_k(x_p) / u_k(x_{p+1}), \quad (2.5)$$

equation (2.3) turns out to be a recurrence relation for  $R_p$ :

$$R_{p-1} = b_p(\epsilon) - 1/R_p. \quad (2.6)$$

The translational symmetry of  $u_k(x)$  gives rise to the conditions

$$u_k(x_0) = u_k(x_{n+1}) \quad (2.7)$$

and

$$u_k(x_0) / u_k(x_1) = u_k(x_{n+1}) / u_k(x_{n+2}). \quad (2.8)$$

This last requirement can readily be expressed as

$$R_0 = R_{n+1}. \quad (2.9)$$

From the recurrence relations (equation (2.6)), this condition can be expanded by means of a continued fraction

$$R_0 = b_1(\epsilon) - \frac{1}{b_2(\epsilon) - \frac{1}{b_3(\epsilon) - \dots - \frac{1}{b_{n+1}(\epsilon) - 1/R_0}}}. \quad (2.10)$$

It is interesting to realise that this relation does not involve a specific value of the wavenumber  $k$ . This expression will be the basis for the determination of the allowed energy bands without explicitly solving the problem of the band structure. Equation (2.10) can be written as a second-degree equation for  $R_0$ ,

$$B_n(\epsilon)R_0^2 - (B_{n-1}(\epsilon) + A_{n+1}(\epsilon))R_0 + A_n(\epsilon) = 0, \quad (2.11)$$

in which the polynomials  $A_n(\epsilon)$  and  $B_n(\epsilon)$  are generated by the recurrence relations (Wall 1967)

$$A_n(\epsilon) = b_n(\epsilon)A_{n-1}(\epsilon) - A_{n-2}(\epsilon), \quad (2.12)$$

$$B_{n-1}(\epsilon) = b_n(\epsilon)B_{n-2}(\epsilon) - B_{n-3}(\epsilon), \quad (2.13)$$

with the following initial values:

$$A_0(\epsilon) = 1, \quad A_1(\epsilon) = b_1(\epsilon), \quad (2.14)$$

$$B_0(\epsilon) = 1, \quad B_1(\epsilon) = b_2(\epsilon). \quad (2.15)$$

The discriminant of the second-degree equation (2.11) will appear as a crucial quantity in further developments. By use of the determinant formula (Wall 1967)

$$A_n(\epsilon)B_n(\epsilon) - A_{n+1}(\epsilon)B_{n-1}(\epsilon) = 1, \quad (2.16)$$

this discriminant is written in the form

$$\Delta = (A_{n+1}(\epsilon) - B_{n-1}(\epsilon))^2 - 4. \quad (2.17)$$

Let us now apply the condition (2.7). It is straightforward that  $u_k(x_0)$  is related to  $u_k(x_{n+1})$  by the relation

$$u_k(x_0) = \left( \prod_{p=0}^n R_p \right) e^{ikL} u_k(x_{n+1}), \quad (2.18)$$

where  $L = x_{n+1} - x_0$  is the period of the potential. To impose the periodic condition (2.7) then amounts to requiring that

$$\prod_{p=0}^n R_p = e^{-ikL} \quad (2.19)$$

It is important to notice that the left-hand side of equation (2.19) depends only on the energy  $\epsilon$  and not explicitly on the wavenumber  $k$ . Allowed bands correspond to the energy ranges for which some real value of  $k$  satisfies equation (2.19). This happens if and only if

$$\left| \prod_{p=0}^n R_p \right| = 1. \quad (2.20)$$

We will now show that this condition is equivalent to the requirement that the discriminant  $\Delta$  of equation (2.11) is negative or zero, i.e.

$$(A_{n+1}(\epsilon) - B_{n-1}(\epsilon))^2 - 4 \leq 0. \quad (2.21)$$

The proof of this is straightforward if one uses the simple relation

$$\prod_{p=0}^n R_p = B_n(\epsilon)R_0 - B_{n-1}(\epsilon) \quad (2.22)$$

demonstrated in the Appendix. Owing to this relation, the left-hand side of equation (2.19) is directly connected with the solutions of the second-degree equation (2.11).

When  $\Delta$  is strictly negative, both roots of this equation are complex conjugate:

$$R_0 = \frac{A_{n+1}(\epsilon) + B_{n-1}(\epsilon)}{2B_n(\epsilon)} \pm i \frac{[4 - (A_{n+1}(\epsilon) - B_{n-1}(\epsilon))^2]^{1/2}}{2B_n(\epsilon)}. \quad (2.23)$$

These solutions are introduced in equation (2.22) to provide a closed expression for the product (2.22):

$$\prod_{p=0}^n R_p = P_{n+1}(\epsilon) \pm i [1 - (P_{n+1}(\epsilon))^2]^{1/2}. \quad (2.24)$$

The polynomial  $P_{n+1}(\epsilon)$  appearing in this expression is given by

$$P_{n+1}(\epsilon) = \frac{1}{2}(A_{n+1}(\epsilon) - B_{n-1}(\epsilon)). \quad (2.25)$$

The formulation (2.24) explicitly shows that the left-hand side of equation (2.19) satisfies equation (2.20).

Alternatively, if  $\Delta$  is strictly positive, both roots of equation (2.11) are real and

$$\prod_{p=0}^n R_p = P_{n+1}(\epsilon) \pm [(P_{n+1}(\epsilon))^2 - 1]^{1/2}. \quad (2.26)$$

In this case the product (2.22) is real and different from  $\pm 1$ .

If  $\Delta$  is equal to zero, i.e.

$$P_{n+1}(\epsilon) = \pm 1, \quad (2.27)$$

one has respectively

$$\prod_{p=0}^n R_p = \pm 1. \quad (2.28)$$

To summarise, when  $\Delta$  is negative or zero,  $|\prod_{p=0}^n R_p| = 1$  and the dispersion relation (2.19) admits real solutions  $k$ : the corresponding energy  $\epsilon$  is then allowed. Otherwise ( $\Delta > 0$ ),  $\prod_{p=0}^n R_p$  is a real number different from  $\pm 1$ , and  $k$  can only be imaginary: the selected energy level  $\epsilon$  is then forbidden. The alternation of allowed and forbidden energy bands is closely related to the sign variations of the discriminant  $\Delta$ . The band edges correspond to the zeros of this discriminant. These can be evaluated by means of a standard roots-finder algorithm. One of the best routines presently available is described by Forsythe *et al* (1977). The discriminant can easily be computed for any value of the energy by means of the recurrence relations (2.12)–(2.15).

The above discussion answers question (i) that was posed at the opening of this section. The answer to question (ii), about the computation of the dispersion law, now follows in a straightforward way. Let us first notice that this dispersion relation can be restricted to the Brillouin zone extending from  $k = -\pi/L$  to  $k = \pi/L$ . Indeed, the right-hand side of equation (2.19) is a periodic function of  $k$  with a period  $2\pi/L$ .

Similarly, the inversion symmetry of the dispersion law  $\epsilon(k) = \epsilon(-k)$  is also conserved. This is due to the fact that, for each allowed energy value  $\epsilon$ , equation (2.11) has two complex conjugate solutions  $R_0$  and  $R_0^*$ . These roots generate from equation (2.22) two dispersion relations for the same energy:

$$\prod_{p=0}^n R_p(\epsilon) = e^{-ikL} \quad (2.29)$$

and

$$\prod_{p=0}^n R_p^*(\epsilon) = e^{-ikL} \quad (2.30)$$

Both relations can be transformed among each other by an inversion in  $k$  space. A twofold degeneracy is then rediscovered. It corresponds to the opposite directions of the travelling waves. In connection with this interpretation, we may notice that the discretised form of the current probability at the point  $x_0$  is given by

$$j(x_0) = -(2/\hbar) |\psi(x_1)|^2 \text{Im } R_0. \quad (2.31)$$

Changing the sign of the imaginary part of the quantity  $R_0$  thus inverts the current probability.

Equation (2.19) gives the dispersion relation in the form  $k = k(\epsilon)$ . However, because inside an allowed energy band equation (2.24) is always true, this equation is strictly equivalent to the more simple formulation

$$\cos kL = P_{n+1}(\epsilon). \quad (2.32)$$

The band structure calculation only needs the evaluation of the polynomial (2.25) by means of the recurrence relations (2.12)–(2.15).

### 3. Examples

In this section we compare the numerical results obtained by using the method described in this paper with an exactly solvable case. The potential considered is

$$v(x) = 2 \cos 2x, \quad (3.1)$$

having a period  $\pi$  and leading to the well-known Mathieu equation (Campbell 1955). The allowed energy bands are most often referred to as 'stable regions' and are quite well known. Table 1 compares the values produced by equation (2.21) with the correct values of the two lower-energy bands. The number of points in the subdivision has been taken equal to 50, 100 and 300. It can be noticed that good accuracy is obtained, even if the discretisation step is not extremely small. Equation (2.32) has been used to determine the dispersion relation. The results are plotted in figure 1 for the lowest bands. Comparison of the numerical results with the dispersion relation of the Mathieu equation shows that the relative discrepancies are never larger than  $5 \times 10^{-3}$  for a subdivision of 50 points.

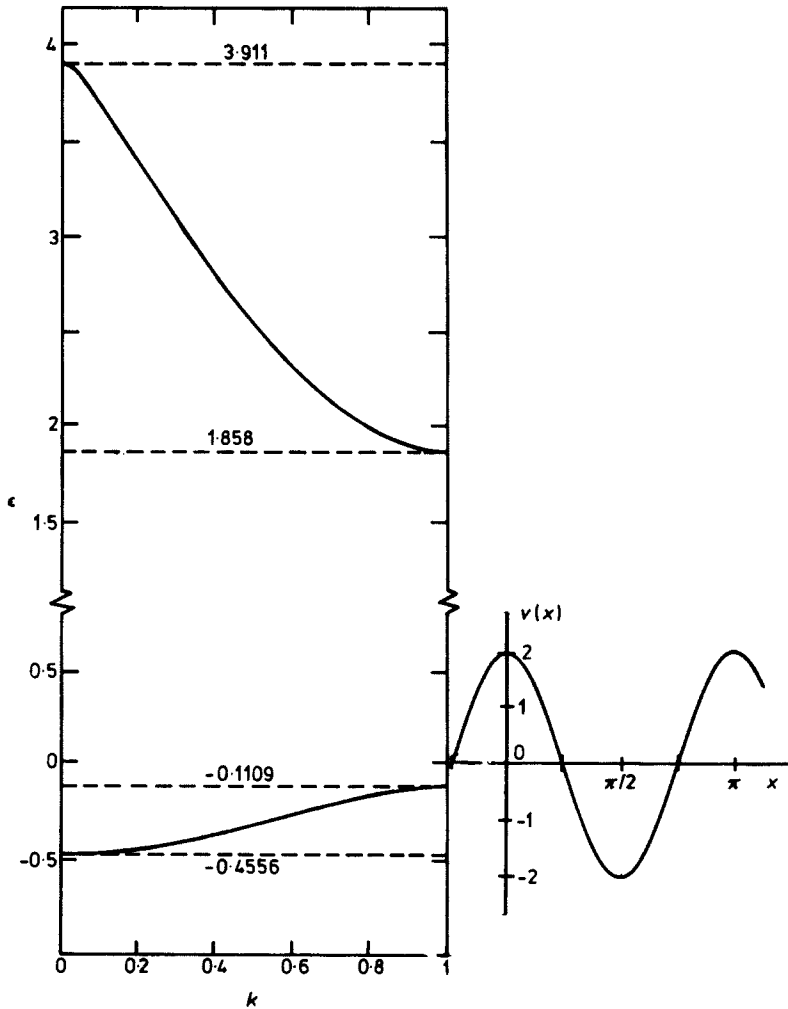
**Table 1.** Comparison of band limits produced by applying relation (2.21) for 50, 100 and 300 points of subdivision in the case of a periodic potential  $v(x) = 2 \cos 2x$ .  $\epsilon(\text{exact})$  are results based on analytic properties of the Mathieu equation.

	$\epsilon(\text{exact})$	$\epsilon(n = 50)$	$\epsilon(n = 100)$	$\epsilon(n = 300)$
Upper band	3.917 02 1.859 11	3.911 1.858	3.9156 1.8589	3.9169 1.859 08
Lower band	-0.110 249 -0.455 139	-0.1109 -0.4556	-0.110 41 -0.455 27	-0.110 266 -0.455 153

As a second example we have solved the Kronig-Penney equation (figure 2) and have reached the same order of accuracy. In this example, care must be paid to the potential discontinuities. It can be shown that, in order to keep a uniform convergence rate (proportional to  $h^2$ ), the potential at these points must be defined as the arithmetic mean of the left and right limiting values. Moreover, the step size  $h$  must be such that the discontinuities are located on some grid points.

### 4. Conclusions

In this paper a numerical approach for a general periodic one-dimensional Schrödinger equation is discussed. This method is based on a discretisation of the derivative operator appearing in the Hamiltonian, which reduces the problem to an eigenvalue equation for a second-order difference operator. This new problem can easily be handled by means of the theory of continued fractions. An equation is provided to determine the location and width of the band gaps, and the band structure is obtained as an explicit expression of the Bloch wavevector as a function of the energy. Some examples have been considered in order to shed some light on the efficiency of the



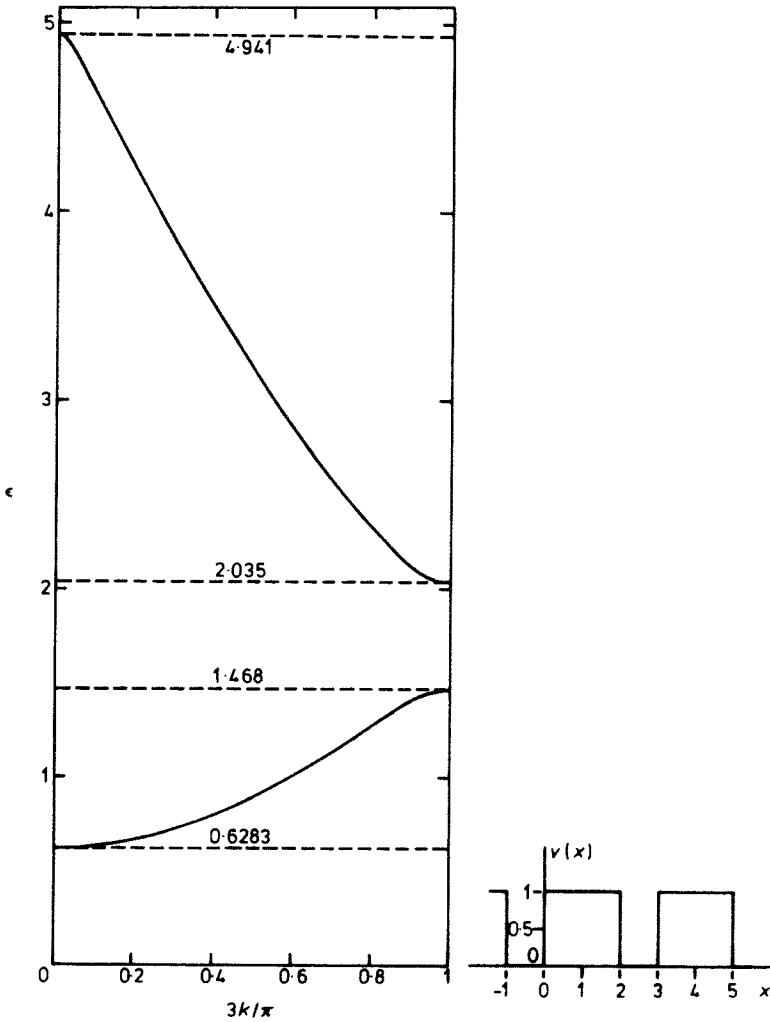
**Figure 1.** Band structure arising from a periodic potential of the form  $v(x) = 2 \cos 2x$ . The Schrödinger equation considered reduces in this case to the Mathieu equation. This result is obtained from equation (2.32) with  $n = 50$ .

general method. The accuracy obtained is already good for a reasonable number of points in the discretisation grid (say 50), and the relative discrepancy with the eigenvalues of the differential operator decreases in proportion to the second power of the step size. This rate of convergence is reasonable for most applications.

The possibility of computing the wavefunction has not been described explicitly in the present paper. This calculation is never really needed for obtaining the energies, but, for some physical applications, the wavefunctions can be easily generated from relations (2.5), (2.6) and (2.11) for Bloch states, once the energies or band structures have been determined.

It is quite interesting to notice that the discrete approximation conserves the more relevant properties of the problem, such as the existence of bands and gaps, the periodicity of the energy in  $k$  space, or the fact that  $\epsilon(k)$  is an even function of  $k$ . This





**Figure 2.** Band structure for a Kronig-Penney model. Equation (2.32) has been used with  $n = 50$ .

seems to indicate that the approach considered here is very well suited to this particular situation.

For the future, many possible extensions of this work can be considered. One of them, which seems to be quite straightforward, is the consideration of a variable step in the discretisation scheme. This does not affect drastically the basic relation (2.10) except that the values of the step sizes  $x_{p+1} - x_p$  and  $x_p - x_{p-1}$  will affect the coefficients of the continued fraction. However, the choice of the local value of the step for a given potential is a delicate question, and designing an adaptative algorithm does not seem very easy.

Perhaps a more straightforward improvement would be to use the Numerov discretisation scheme (Numerov 1924) rather than the simple one discussed here. This more sophisticated scheme (with a truncation error proportional to  $h^4$ ) is readily applicable here.

However, the simple method described in this paper has the advantage of being very easily implemented. The computation time and storage are so reduced that even most common programmable pocket calculators can be used to perform the band structure calculation.

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### Appendix

In this Appendix we prove the relation

$$\prod_{p=0}^n R_p = B_n(\epsilon)R_0 - B_{n-1}(\epsilon). \quad (\text{A1})$$

This proof can be reached in two steps. The first one consists of deriving the following formula by a recurrence scheme:

$$\prod_{p=0}^n R_p = A_n(\epsilon)R_n - A_{n-1}(\epsilon). \quad (\text{A2})$$

For  $n = 1$  this relation is evident from equation (2.6), and the particular values of  $A_1(\epsilon)$  and  $A_0(\epsilon)$  given by (2.14). If we suppose that equation (A2) is true for  $n = k - 1$ , then for  $n = k$  we can write

$$\prod_{p=0}^k R_p = \prod_{p=0}^{k-1} R_p R_k \quad (\text{A3})$$

$$= A_{k-1}(\epsilon)R_{k-1}R_k - A_{k-2}(\epsilon)R_k. \quad (\text{A4})$$

By using again equation (2.6) one can transform this last result into

$$\prod_{p=0}^k R_p = (A_{k-1}(\epsilon)b_k - A_{k-2}(\epsilon))R_k - A_{k-1}(\epsilon). \quad (\text{A5})$$

Relation (A2) then follows in a straightforward way from the recurrence relation defining the polynomial  $A_k(\epsilon)$  (equation (2.12)).

The second step will lead to the completion of the proof of equation (A1). The recurrence relation (2.6) can be once again used to derive an equivalent form of equation (A2):

$$\prod_{p=0}^n R_p = A_{n+1}(\epsilon) - \frac{A_n(\epsilon)}{R_{n+1}}. \quad (\text{A6})$$

The periodic condition (2.9) readily yields

$$\prod_{p=0}^n R_p = \frac{A_{n+1}(\epsilon)R_0 - A_n(\epsilon)}{R_0}. \quad (\text{A7})$$

Now,  $R_0$  satisfies the second-degree equation (2.11), which can be written as

$$A_{n+1}(\epsilon)R_0 - A_n(\epsilon) = (B_n(\epsilon)R_0 - B_{n-1}(\epsilon))R_0. \quad (\text{A8})$$

Relation (A1) is then obvious.

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