A transfer matrix method for the determination of one-dimensional band structures

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Abstract. We show that the discretized forms of the Schrödinger and the Dirac equations for an arbitrary potential in one dimension are equivalent to the Poincaré map of the corresponding wave equation for an array of δ-function potentials. Therefore, the dynamics of particles in general periodic potentials may be studied by means of an equivalent generalized Kronig–Penney model, in which there exist several δ-function potentials in each unit cell. Taking into account the techniques of dynamical systems, the transfer matrix method is then used in a simple form to compute the energy band edges and the dispersion law inside the allowed bands.

1. Introduction

One-dimensional physical models (Lieb and Mattis 1966, Bernasconi and Schneider 1981, Albeverio *et al* 1988, and references therein) play an important role in understanding the quantum mechanics of electrons in perfect and non-perfect lattices. Some important concepts in electron dynamics in periodic lattices, such as Bloch states and the occurrence of energy bands and gaps, as well as in disordered lattices, such as localization and the existence of mobility edges, are now well understood with the aid of one-dimensional models. Of course, these models are far from giving a complete account of the number of situations occurring in real crystals. Some limitations are not directly related to the dimensionality of the problem but to the potential model used in describing the electron interaction with the crystal. It is clear that an array of square-well or δ-function potentials (Kronig and Penney 1931) is a crude picture of the electron interaction with other electrons and atoms in a solid. One method to overcome this difficulty is to use non-local separable potentials, which admit exact solutions for an arbitrary potential shape (Domínguez-Adame *et al* 1991, Domínguez-Adame and González 1992). Moreover, numerical solutions of the wave equation corresponding to a general periodic potential give accurate results when analytical solutions are absent. At present there exist numerical methods for one-dimensional band calculations based on the discretized Schrödinger (Vigneron and Lambin 1979) and Dirac equations (Méndez and Domínguez-Adame 1991). These methods use a continued fraction approach to compute the energy band edges and dispersion relations inside the allowed bands.

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The aim of this paper is to present an alternative numerical method to study the dynamics of non-relativistic and relativistic electrons in one-dimensional potentials. We will show that the discretized forms of the Schrödinger (section 2) and Dirac equations (section 3) can be replaced by the Poincaré map associated with the corresponding wave equation for an array of δ-function potentials, within the same truncation error as that of the original discretization scheme. In the case of general periodic potentials, the problem is equivalent to the generalized Kronig-Penney or Dirac–Kronig–Penney models with the same period as that of the original potential. This replacement will allow us to use the transfer matrix technique for the computation of the dispersion law. Some numerical results are presented in section 4; the convergence of the method is discussed and non-relativistic and relativistic band structures are compared. The main conclusions of the present work are drawn in section 5.

2. Non-relativistic electrons in periodic potentials

We start with the one-dimensional Schrödinger equation for steady states ($\hbar = 2m = 1$)

$$\left[-\frac{d^2}{dx^2} + V(x) \right] \psi(x) = E\psi(x) \tag{1}$$

$V(x)$ being a general potential. Let us divide the interval $[a, b]$ into $N+1$ equal parts of length $h = (b-a)/(N+1)$, which defines the grid $x_n = nh + a$ ($n = 0, 1, \ldots, N+1$). The discretized form of (1) at any point of the grid is

$$\psi_{n+1} + \psi_{n-1} = (2 - h^2 E + h^2 V_n)\psi_n \tag{2}$$

with a truncation error proportional to h^2. Here $\psi_n \equiv \psi(x_n)$ and $V_n \equiv V(x_n)$. In the case of periodic potentials satisfying the condition $V(x) = V(x+L)$, L being the period, we take $a = 0$ and $b = L$ so that $[0, L]$ denotes the unit cell of the crystal. Since the Bloch theorem must be satisfied, the wavefunction is of the form $\psi(x+L) = \exp(\mathrm{i}kL)\psi(x)$ and the boundary condition for the difference equation reads

$$\psi_{n+N+1} = \exp(\mathrm{i}kL)\psi_n. \tag{3}$$

In order to solve (2) and (3) we consider a periodic array of equally spaced δ-function potentials, and let h be the distance between nearest-neighbour sites. The interaction of an electron of mass $m = \frac{1}{2}$ with this potential obeys the following Schrödinger equation

$$\left[-\frac{d^2}{dx^2} + \sum_n \lambda_n \delta(x - nh) \right] \psi(x) = E\psi(x) \tag{4}$$

where λ_n is the potential strength of the nth site. We can now use the techniques of dynamical systems proposed by Bellisard *et al* (1982) to construct the Poincaré map associated with (4), obtaining

$$\psi_{n+1} + \psi_{n-1} = [2 \cos(h\sqrt{E}) + \lambda_n \sin(h\sqrt{E})/\sqrt{E}]\psi_n. \tag{5}$$

$\psi_n \equiv \psi(x_n)$ is well defined since $\psi(x)$ is a continuous function at the points where the δ-function potentials are located, although its derivative is discontinuous. We stress the fact that nothing has been lost when passing from (4) to (5), and (5) contains all the band structure information. In the limit $h \to 0$, when δ-function potentials are closely spaced, (5) reduces to

$$\psi_{n+1} + \psi_{n-1} = (2 - h^2 E + h\lambda_n)\psi_n \tag{6}$$

with a truncation error of the order of h^2. This approximation becomes valid provided that $h\sqrt{E} \ll 1$. We note that (6) is equivalent to our original problem (2) if we take

$$\lambda_n = hV_n. \tag{7}$$

Therefore, the strength of the nth δ-function potential depends on the value of the periodic potential $V(x)$ at the nth site. Since $V_{n+N+1} = V_n$, the array of δ-function potentials in (4) becomes periodic of period $h(N+1) = L$ and the boundary condition (3) also applies to (6).

The equation (4) corresponds to a Kronig–Penney model for a polyatomic crystal, the so-called generalized Kronig–Penney model (Roy and Bhattacharya 1969, Eldib *et al* 1987). Each 'atom' of the unit cell $[0, L]$, represented by a δ-function potential, is separated an equal distance h apart from its nearest neighbours. Instead of (4), we use equation (6) since it gives the same results with an error of the order of h^2, which is the same error of passing from (1) to (2). One can find the dispersion relation of the generalized Kronig–Penney model by means of the transfer matrix technique, in analogy to the usual tight-binding model. In (6) the hopping energy between nearest neighbours is constant, so we are dealing with a diagonal tight-binding model. In that case, the transfer matrix takes a simple form

$$\begin{pmatrix} \psi_{n-1} \\ \psi_n \end{pmatrix} = \begin{pmatrix} 2 + \lambda_n h - h^2 E & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \psi_n \\ \psi_{n+1} \end{pmatrix} \equiv P_n \begin{pmatrix} \psi_n \\ \psi_{n+1} \end{pmatrix} \tag{8}$$

with $\det(P_n) = 1$. Iterating (8) and using the boundary condition (3) we find

$$\begin{pmatrix} \psi_0 \\ \psi_1 \end{pmatrix} = P_1 P_2 \dots P_{N+1} \begin{pmatrix} \psi_{N+1} \\ \psi_{N+2} \end{pmatrix} \equiv T_{N+1} \exp(ikL) \begin{pmatrix} \psi_0 \\ \psi_1 \end{pmatrix} \tag{9}$$

where T_{N+1} is the transfer matrix for the unit cell. Requiring the determinant to vanish for non-trivial solutions we get

$$\cos(kL) = \tfrac{1}{2} \mathrm{Tr}(T_{N+1}) \equiv F_{N+1}(E). \tag{10}$$

The required symmetry of the dispersion relation $E(k) = E(-k)$ is conserved. Real values of k give the dispersion relation inside the allowed bands, whereas the energy band edges are computed through the condition $|F_{N+1}(E)| = 1$. The trace of the transfer matrix may be calculated recursively. Starting from the fact that $T_{N+1} = T_N P_{N+1}$, we find the following recurrence relations for the diagonal terms of the transfer matrices

$$(T_{N+1})_{11} = (2 + \lambda_{N+1}h - h^2 E)(T_N)_{11} - (T_{N-1})_{11} \tag{11a}$$

$$(T_{N+1})_{22} = (2 + \lambda_N h - h^2 E)(T_N)_{22} - (T_{N-1})_{22} \tag{11b}$$

with the initial conditions $(T_0)_{11} = (T_0)_{22} = 1$, $(T_1)_{11} = 2 + \lambda_1 h - h^2 E$ and $(T_1)_{22} = 0$. If we restrict ourselves to the case of smooth potentials and small h, the following approximated recurrence relation for $F_{N+1}(E)$ is valid

$$F_{N+1}(E) = (2 + \lambda_{N+1}h - h^2 E)F_N(E) - F_{N-1}(E) \tag{12}$$

where now the initial conditions are $F_0(E) = 1$ and $F_1(E) = 1 + \lambda_1 h/2 - h^2 E/2$.

3. Relativistic electrons in periodic potentials

In this section we aim to show that the above treatment may be generalized for Dirac electrons. Let us consider the one-dimensional Dirac equation for an electron of mass

$m = \frac{1}{2}$ in a periodic potential $V(x)$ of period L. In units $\hbar = c = 1$ we write

$$\left[-i\alpha \frac{d}{dx} + \tfrac{1}{2}\beta + V(x) \right] \psi(x) = E_R \psi(x) \tag{13}$$

where $\psi(x)$ is the two-component wavefunction, α and β are 2×2 traceless, Hermitian matrices with square unity, and E_R is the relativistic energy of the electron. To solve the Dirac equation we set the representation $\alpha = \sigma_z$ and $\beta = \sigma_x$, σs being the Pauli matrices. Defining $E \equiv E_R - \frac{1}{2}$ and denoting by ϕ and χ the upper and lower components of the wavefunction, respectively, we obtain

$$\chi(x) = 2\left[i\frac{d}{dx} - E + V(x) + \tfrac{1}{2} \right] \phi(x) \tag{14}$$

$$\left[\frac{d^2}{dx^2} + V^2(x) + E(E+1) - (2E+1)V(x) - i\frac{dV(x)}{dx} \right] \phi(x) = 0. \tag{15}$$

We restrict ourselves to a smooth potential hereafter, so we neglect the term dV/dx in (15). The discretized version of (15) reads as follows

$$\phi_{n+1} + \phi_{n-1} = [2 - h^2(V_n^2 + E(E+1) - (2E+1)V_n)]\phi_n. \tag{16}$$

Since $V_{n+N+1} = V_n$ the Bloch theorem holds and leads to

$$\phi_{n+N+1} = \exp(ikL)\phi_n \tag{17}$$

and (14) ensures that χ is also a Bloch function.

Following the same procedure as before, we consider the Dirac equation for a periodic array of δ-function potentials

$$\left[-i\sigma_z \frac{d}{dx} + \tfrac{1}{2}\sigma_x + \sum_n \lambda_n \delta(x - nh) \right] \psi(x) = (E + \tfrac{1}{2})\psi(x). \tag{18}$$

Taking into account that the appropriate boundary condition for a (electrostatic-like) δ-function potential located at x_n reads (McKellar and Stephenson 1987, Domínguez-Adame and Maciá 1989) as

$$\psi(x_n^+) = (\cos \lambda_n - i\sigma_z \sin \lambda_n)\psi(x_n^-) \tag{19}$$

we have obtained the Poincaré map associated with (18) in the representation we have chosen

$$\phi_{n+1} + \exp(i\lambda_n - i\lambda_{n-1})\phi_{n-1}$$
$$= [2\cos\lambda_n \cos(\sqrt{E(E+1)}h)$$
$$+ (2E+1)\sin\lambda_n \sin(\sqrt{E(E+1)}h)/\sqrt{E(E+1)}]\phi_n \tag{20}$$

where $\phi_n = \phi(n^-h)$ (note that $\phi(x)$ is not continuous at $x = nh$, according to (19)). It is worthwhile mentioning that (20) gives the same band structure as (18). In particular, in the case with $\lambda_n = \lambda$, the whole band structure of the Dirac–Kronig–Penney model (Méndez and Domínguez-Adame 1992) is recovered. In the limit $h \to 0$ and for smooth potentials ($\lambda_n/\lambda_{n-1} \ll 1$) we have

$$\phi_{n+1} + \phi_{n-1} = [2 - (\lambda_n^2 + E(E+1)h^2 - (2E+1)\lambda_n h)]\phi_n. \tag{21}$$

Hence (21) becomes equivalent to (16) by the substitution $\lambda_n = hV_n$. As occurs in the non-relativistic case, the periodic boundary condition (17) also applies to (21). Note

that (21) reduces to (6) in the non-relativistic and weak coupling limits, as $E \ll \frac{1}{2}$ and $V_n \ll \frac{1}{2}$. Equation (18) corresponds to the so-called generalized Dirac–Kronig–Penney model (Domínguez-Adame 1989), in which there are several 'atoms' in the unit cell $[0, L]$. This model is also exactly solvable and we can again use the transfer matrix technique.

Following the same procedure as before, we find that the dispersion law is also given by (10), but now the diagonal elements of the transfer matrices obey the following recurrence relationship

$$(T_{N+1})_{11} = [2 + (2E+1)\lambda_{N+1}h - E(E+1)h^2 - \lambda_{N+1}^2](T_N)_{11} - (T_{N-1})_{11} \qquad (22a)$$

$$(T_{N+1})_{22} = [2 + (2E+1)\lambda_N h - E(E+1)h^2 - \lambda_N^2](T_N)_{22} - (T_{N-1})_{22} \qquad (22b)$$

with the initial conditions $(T_0)_{11} = (T_0)_{22} = 1$, $(T_1)_{11} = 2 + (2E+1)\lambda_1 h - E(E+1)h^2 - \lambda_1^2$ and $(T_1)_{22} = 0$. For large N values we find that $F_{N+1}(E)$ may be approximately evaluated from the relation

$$F_{N+1}(E) = [2 + (2E+1)\lambda_{N+1}h - E(E+1)h^2 - \lambda_{N+1}^2]F_N(E) - F_{N-1}(E) \qquad (23)$$

with $F_0(E) = 1$ and $F_1(E) = 1 + (E + \frac{1}{2})\lambda_1 h - E(E+1)h^2/2 - \lambda_1^2/2$.

4. Numerical results

As an example of this method, we have studied numerically the Mathieu potential

$$V(x) = V_0 \cos(2\pi x/L)$$

for both non-relativistic and relativistic particles of mass $m = 0.5$. We take $L = \pi$ hereafter. The Schrödinger equation for the Mathieu potential is exactly solvable, so we can use the analytic solutions to check the numerical solutions. Unfortunately there are no analytical results in the case of the Dirac equation. We have found in our studies that good accuracy is obtained even if a small number of grid points is used ($N = 50$ or 100). Comparison of non-relativistic band limits produced by applying (10) and (11) with exact results is presented in table 1 when $V_0 = 2$. Notice that results are improved by means of the Richardson extrapolation formula, where the corresponding energy value is given as $(4E(2N) - E(N))/3$, $E(N)$ being the value obtained with N subdivisions in the interval (in our case we have taken $N = 300$). In the case of the Dirac equation accurate results are also usually found taking about 50–100 grid points. However, the number of these points has to be greater to calculate the dispersion relation for higher bands. Figure 1 shows the dispersion relation for both non-relativistic

Table 1. Band limits for a non-relativistic particle of mass $m = 0.5$ in the potential $V(x) = V_0 \cos 2x$, with $V_0 = 2$. N indicates the number of grid points. Energy values obtained by the Richardson rule are also shown. Exact values are based on the analytic properties of the Mathieu solutions.

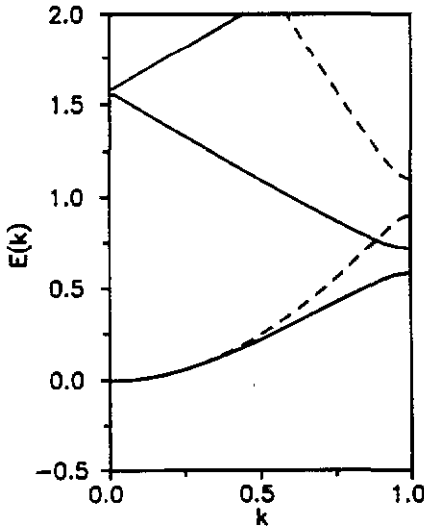|	$N = 50$	$N = 300$	$N = 600$	Richardson	Exact
Upper band	3.911 446	3.916 865	3.916 986	3.917 026	3.917 017
	1.858 290	1.859 084	1.859 102	1.859 108	1.859 107
Lower band	−0.110 874	−0.110 266	−0.110 253	−0.110 249	−0.110 249
	−0.455 660	−0.455 153	−0.455 142	−0.455 138	−0.455 139

Figure 1. Non-relativistic (dashed line) and relativistic (solid line) band structures for a particle of mass $m = 0.5$ in the potential $V(x) = V_0 \cos 2x$, with $V_0 = 0.2$. The number of points in the subdivision is $N = 200$.

and relativistic particles in the case $V_0 = 0.2$ and $N = 200$. As expected, marked differences appear because the potential is rather strong ($V_0 = 2m/5$ being of order of the rest-mass energy of the particle). We observe that relativity causes the shrinkage of the spectrum (for more details see Méndez and Domínguez-Adame 1991 and references therein). In contrast to the continued fraction approach to relativistic band structures of Méndez and Domínguez-Adame (1991), our transfer matrix method does not require the potential to be symmetric around atomic positions. Therefore, this method is applicable to more general periodic potentials, often used in semiconductor superlattices calculations (sawtooth potentials, etc).

5. Conclusions

In this paper we have demonstrated that the dynamics of both non-relativistic and relativistic particles in general one-dimensional potentials is equivalent to the dynamics of particles in an array of δ-function potentials. In our opinion this is an interesting result because this equivalence explains why the Kronig–Penney model (periodic, quasiperiodic or random) works so well in explaining the electron behaviour in real lattices. In the case of a general periodic potential we have found that the dispersion relation is the same as that of a generalized Kronig–Penney model. The transfer matrix technique allows us to obtain a very simple recursive method to compute $E(k)$. The computation time and storage are much reduced so that this method may be implemented by most programmable pocket calculators. In addition, it possesses the advantage that other numerical methods widely used in tight-binding calculations (recall that (6) and (21) are essentially identical to a tight-binding Hamiltonian) may be extended straightforwardly to be applied in our calculations. In particular, the negative-eigenvalue theory of Dean (1972) provides a simple scheme for the determination of

the density of states without the knowledge of the dispersion relation inside allowed bands.

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