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# The Kronig–Penney lattice with $R$ matrix interactions

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**Abstract.** The Kronig–Penney lattice is a one-dimensional chain of equal segments at the end of which there is a  $\delta$  function interaction. It predicts for the energy a band structure whose width increases with the energy. These results continue to hold when the  $\delta$  functions are replaced by arbitrary potentials, as well as when the problem is generalized to three dimensions giving the well known conduction bands for electrons. In this paper we are interested in what happens to neutrons in crystals. The simplest model would again be a Kronig–Penney lattice, but with the  $\delta$  function replaced by boundary conditions at the end of the segments. This approach leads to an  $R$  matrix interaction of the type Wigner introduced in his analysis of nuclear reactions. Using Bloch's theorem we solve the problem of the band structure for arbitrary  $R$ , but discuss its behaviour only when it has a single pole, a pole and a zero or a picket-fence form. An example with data taken from experiment is presented in the appendix.

## 1. Introduction

The Kronig–Penney [1] one-dimensional lattice has been very useful as a guide in the study of the energy band structure in the solid state. It consists of blocks of equally spaced identical potentials along a line and, with the help of Bloch's theorem [2], the solution of the stationary Schrödinger equation can be found for the lattice if it is known in one of the blocks.

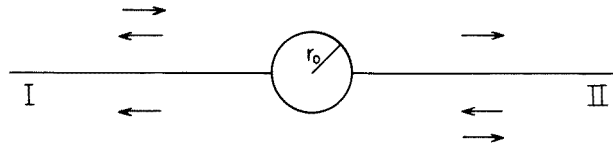
The purpose of this paper is to replace the potential by an interaction of the  $R$  matrix form at the end of each block. This has already been done in a one-dimensional problem with an  $R$  matrix at the origin and with a single pole, for the purpose of discussing the delay time for a single resonance [3]. Instead of discussing the time-dependent problem as was done in [3], we shall deal with the stationary problem but with  $R$  matrices with several poles and situated at the end of each block.

Before going into the problem itself we review some elementary aspects of Wigner's  $R$  matrix theory, originally developed for nuclear reactions, so as to show how easily it can be incorporated in our lattice problem.

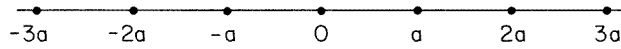
## 2. The Wigner $R$ matrix theory

The concept indicated in the title of this section was developed originally with the purpose of describing nuclear reactions involving neutrons [4], which move as essentially free particles until they come close to a nucleus within the range of nuclear forces. We shall consider the simplest case of an s-wave two-channel reaction illustrated in figure 1. The nucleus is supposed to be surrounded by a sphere of radius  $r_0$  where ingoing and outgoing waves will be spherical

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**Figure 1.** The two channels are indicated by the left and right lines and the internal region is surrounded by the circle. If the incoming particle starts from left the incoming and outgoing waves are indicated by arrows above the line, while in the second channel we have only out going waves. The situation is reversed if we start from the right as indicated by the arrows below the line.



**Figure 2.** A schematic picture of the Kronig-Penney lattice with  $R$  matrix interactions indicated by equally spaced dots.

in shape. We indicate their radial motion by a straight line, where the one on the left describes the first of the channels and the one on the right, the second. In figure 1 on the upper left the arrows  $\rightleftharpoons$  indicate the ingoing and outgoing waves in the first channel. The  $\rightarrow$  on the upper right indicates the outgoing wave for the second channel coming from the left. On the lower part we have the same situation, but reversed.

If the wavefunctions in the first and second channels are indicated respectively by  $\psi_1(r)$ ,  $\psi_2(r)$ , in which the factor  $r$  is already included to simplify the radial form of the Laplacian, Wigner states that the interaction is given by the relation [4]:

$$\begin{bmatrix} \psi_1(r_0) \\ \psi_2(r_0) \end{bmatrix} = \mathbf{R}(E) \begin{bmatrix} \left( \frac{\partial \psi_1}{\partial r} \right)_{r=r_0} \\ \left( \frac{\partial \psi_2}{\partial r} \right)_{r=r_0} \end{bmatrix} \quad (2.1)$$

where  $\mathbf{R}(E)$  is an energy-dependent  $2 \times 2$  matrix whose terms are in turn  $1 \times 1$  i.e. scalar  $\mathbf{R}(E)$  matrices whose general analytic properties we shall discuss later.

Once we have established relations (2.1) we can return to our lattice problem illustrated in figure 2 where the  $\mathbf{R}(E)$  matrix interactions take place at the dots at the end of each block.

### 3. The one-dimensional lattice with $R$ matrix interactions

To begin with we shall use units in which

$$\hbar = m = a = 1 \quad (3.1)$$

where  $m$  is the mass of the particles moving in the lattice and  $a$  is the dimension of each block. We then concentrate on one given point of the lattice, say  $x = 0$ . We then have a two-channel problem because at the left and right of  $x = 0$  we have wavefunctions which we could denote respectively as  $\psi_-(x)$ ,  $\psi_+(x)$ , that at  $x = 0$  take the values  $\psi_-(0)$ ,  $\psi_+(0)$ . We, of course, also have the derivatives of these wavefunctions  $[\partial \psi_-(x)/\partial x]$ ,  $[\partial \psi_+(x)/\partial x]$  but before evaluating them at 0 and establishing a relation of the type (2.1) in  $\mathbf{R}(E)$  matrix theory, we require some caution. In (2.1) the derivative  $\partial/\partial r$  is equivalent  $\mathbf{n} \cdot \nabla$  where  $\mathbf{n}$  is the normal to the spherical surface going *outward*. If it went *inward* obviously we had to use  $-\partial/\partial r$ .

In the lattice problem  $\mathbf{n}$  is the normal of the plane perpendicular to  $x$  and thus  $\mathbf{n} \cdot \nabla$  is  $\partial/\partial x$  for  $\psi_+(x)$  and  $-\partial/\partial x$  for  $\psi_-(x)$ .

Thus an  $\mathbf{R}$  matrix relation of (2.1) can be written as

$$\begin{bmatrix} \psi_-(0) \\ \psi_+(0) \end{bmatrix} = \mathbf{R}(E) \begin{bmatrix} -\left(\frac{\partial\psi_-}{\partial x}\right)_0 \\ \left(\frac{\partial\psi_+}{\partial x}\right)_0 \end{bmatrix}. \tag{3.2}$$

It is now necessary to examine more closely the structure of the  $2 \times 2$  matrix  $\mathbf{R}(E)$  that can be written as

$$\mathbf{R}(E) = \begin{bmatrix} R_{--}(E) & R_{-+}(E) \\ R_{+-}(E) & R_{++}(E) \end{bmatrix}. \tag{3.3}$$

It seems physically reasonable to assume that, for example,  $\psi_-(0)$  interacts in the same way with the two derivatives that are components of the vector of the right-hand side of (3.2) and this would then imply that

$$R_{--}(E) = R_{-+}(E). \tag{3.4}$$

On the other hand if, from (3.2), we would like to derive the relation that the wavefunction is continuous at the origin, i.e.  $\psi_-(0) = \psi_+(0)$ , which is physically required, then we must have

$$R_{--}(E) = R_{+-}(E) \quad R_{-+}(E) = R_{++}(E). \tag{3.5}$$

Thus we conclude that a physically reasonable  $\mathbf{R}(E)$  matrix interaction in the one-dimensional case is

$$\begin{bmatrix} \psi_-(0) \\ \psi_+(0) \end{bmatrix} = R(E) \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} -\left(\frac{\partial\psi_-}{\partial x}\right)_0 \\ \left(\frac{\partial\psi_+}{\partial x}\right)_0 \end{bmatrix}. \tag{3.6}$$

Now we turn to the mathematical works [5] that tell us that the most general form of an  $R(E)$  function is

$$R(E) = \sum_n \frac{\gamma_n^2}{E_n - E} + R_0 \tag{3.7}$$

where the sum could be finite or infinite and  $E_n$  are real constants, associated with resonances, while the  $\gamma_n^2$  are real and positive and associated with the reduced widths of these resonances [4, 5]. The  $R_0$  is also a constant.

Now by subtracting the first from the second row in equation (3.6) we get

$$\psi_-(0) = \psi_+(0) \tag{3.8}$$

and then we can also rewrite the first row in equation (3.6) as

$$\psi_-(0) + R(E) \left(\frac{\partial\psi_-}{\partial x}\right)_0 = R(E) \left(\frac{\partial\psi_+}{\partial x}\right)_0. \tag{3.9}$$

In the next section we use Bloch’s theorem [2] to express the left-hand side of equations (3.8), (3.9) in terms of wavefunctions with + index but at the point  $x = 1$ , which allows us to find the characteristics of our spectra as functions of  $R(E)$ .

#### 4. The Bloch theorem and the formula of a Kronig–Penney lattice with $R$ matrix interaction

As we see from figure 2 our problem, in the units of (3.1), is invariant under translations by 1 and thus Bloch's theorem [2] is applicable. This implies that the wavefunction, and also its derivatives, when translated by  $n$  remains the same but only multiplied by a phase factor  $\exp(i\kappa n)$ , where  $\kappa$  is the irrep of the translation group.

Considering the left-hand side of equations (3.8), (3.9), we see that in a translation by 1 we have

$$\psi_-(0) = e^{i\kappa} \psi_+(1) \quad (4.1)$$

$$\psi_-(0) + R(E) \left( \frac{\partial \psi_-}{\partial x} \right)_0 = e^{i\kappa} \left[ \psi_+(1) + R(E) \left( \frac{\partial \psi_+}{\partial x} \right)_1 \right]. \quad (4.2)$$

Now in the interval between 0 and 1 the wavefunction, in our units, satisfies the free particle wave equation

$$-\frac{\partial^2 \psi_+}{\partial x^2} = p^2 \psi_+ \quad \text{where} \quad E = \frac{1}{2} p^2 \quad 0 < x < 1 \quad (4.3)$$

together with the boundary conditions following from (3.8), (3.9), (4.1) and (4.2) i.e.

$$\psi_+(0) = e^{i\kappa} \psi_+(1) \quad (4.4)$$

$$R(E) \left( \frac{\partial \psi_+}{\partial x} \right)_0 = e^{i\kappa} \left[ \psi_+(1) + R(E) \left( \frac{\partial \psi_+}{\partial x} \right)_1 \right]. \quad (4.5)$$

Thus from (4.3) we have

$$\psi_+(x) = A e^{ipx} + B e^{-ipx} \quad (4.6)$$

where  $A, B$  are functions of  $\kappa, p$  but not of  $x$ , that must be determined from equations (4.4), (4.5) which give us the relations

$$A + B = e^{i\kappa} [A e^{ip} + B e^{-ip}] \quad (4.7)$$

$$ipR(E)(A - B) = e^{i\kappa} [(A e^{ip} + B e^{-ip}) + ipR(E)(A e^{ip} - B e^{-ip})]. \quad (4.8)$$

We can write equations (4.7) and (4.8) in the form

$$c_{11}A + c_{12}B = 0 \quad c_{21}A + c_{22}B = 0 \quad (4.9)$$

where

$$\begin{aligned} c_{11} &= 1 - e^{i(\kappa+p)} & c_{12} &= 1 - e^{i(\kappa-p)} \\ c_{21} &= ipR(E)[1 - e^{i(\kappa+p)}] - e^{i(\kappa+p)} \\ c_{22} &= ipR(E)[-1 + e^{i(\kappa-p)}] - e^{i(\kappa-p)} \end{aligned} \quad (4.10)$$

and thus a solution for  $A, B$  exists only if the determinant vanishes i.e.

$$c_{11}c_{22} - c_{12}c_{21} = 0 \quad (4.11)$$

which, after multiplication by  $\exp(-i\kappa)$ , gives the equation

$$\cos \kappa = \cos p + \frac{1}{2pR(E)} \sin p. \quad (4.12)$$

The expression (4.12) would be the usual [1] Kronig–Penney one if  $R(E)$  is a constant i.e.  $R(E) = R_0$ , which is allowed by (3.7), but for any other values of the latter it gives very different results, as will be discussed in the following sections.

## 5. Band structure for different values of the $R(E)$ function

Now we will find the values for the momentum  $p$  and the energy  $E = \frac{p^2}{2}$  for which equation (4.12) has solution, i.e. the bands of allowed values of  $p$  and  $E$ . This band structure depends, of course, on the choice of the  $R(E)$  function. We will consider some special schematic cases, leaving for the appendix an example with realistic values of the parameters corresponding to the case of a neutron interacting with the atomic nuclei of a one-dimensional crystal.

### 5.1. $R(E)$ function equal to a constant

According to equation (3.7) the simplest non-trivial form of the  $R(E)$  function is when all terms on the right-hand side of that equation are equal to zero except the last one. Thus  $R(E) = R_0$  and, as we have mentioned, it gives rise to the Kronig–Penney model, where one of the well known characteristics of their band structure is that the more the energy increases the more the width of the gaps of forbidden energies decreases. In the limit  $E \rightarrow \infty$  the gaps reduce to isolated points.

### 5.2. $R(E)$ function with a single pole

The next simple case of equation (3.7) is when all terms on the right-hand side are equal to zero except one of the terms indicated in the sum symbol. Thus the system has a single resonance at the pole  $E = E_0$ , i.e.,

$$R(E) = \frac{\gamma_0^2}{E_0 - E} \quad (5.1)$$

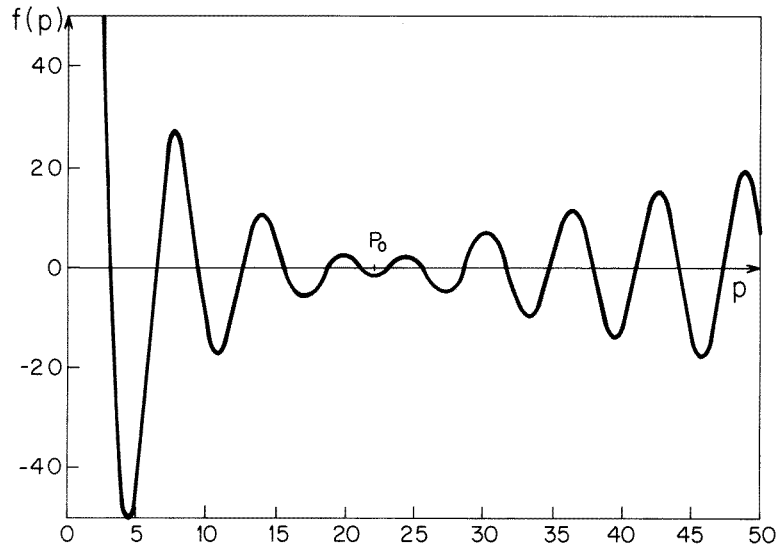
where  $p_0^2 = 2E_0$  and  $p^2 = 2E$ . Therefore the relationship between the index  $\kappa$  and the momentum  $p$  (equation (4.12)) becomes

$$\cos \kappa = \cos p + \frac{p_0^2 - p^2}{4\gamma_0^2} \frac{\sin p}{p}. \quad (5.2)$$

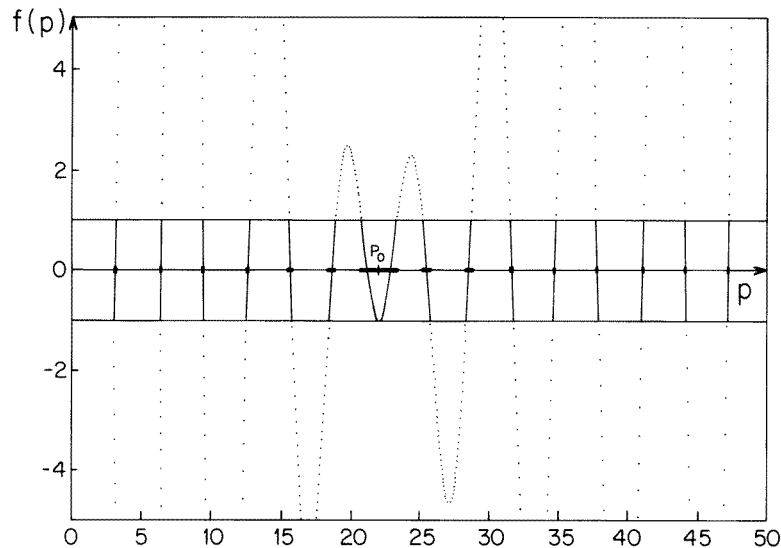
The band structure will be obtained by determining the values of  $p$  for which the above equation has solutions. In order to find these values we will proceed in a similar way as in the usual Kronig–Penney model. Let us consider figures 3 and 4 which are plots of the function  $f(p)$  defined as the right-hand side of equation (5.2):

$$f(p) = \cos p + \frac{p_0^2 - p^2}{4\gamma_0^2} \frac{\sin p}{p} \quad (5.3)$$

for particular values of  $\gamma_0$  and  $p_0$ . Figure 4 is an amplification of figure 3. We have considered only positive values of  $p$  since  $f(p)$  is an even function. We see from equation (5.3) that for large values of  $p$  the amplitude of the oscillations increases linearly with  $p$  as can also be seen in figure 3. However, near the pole  $p_0$ , the second term is very small and the amplitude of the oscillations decreases. Since  $|\cos \kappa| \leq 1$ , equation (5.2) has solutions only for  $p$  values for which the curve of  $f(p)$  lies between the two horizontal lines at the heights  $-1$  and  $1$ , respectively (see figure 4). We will call the region between these two horizontal lines region  $\mathcal{S}$ . The continuous (dotted) curves in figure 4 represent the values of  $f(p)$  which are inside (outside)  $\mathcal{S}$ . The values of  $p$  for which the values of  $f(p)$  are inside  $\mathcal{S}$  are also indicated by the heavy lines on the horizontal axis. These are the  $p$  bands corresponding to this form of  $R(E)$ . It is clear that when the amplitude of  $f(p)$  increases the slope of the curve  $f(p)$  between two adjacent extreme values increases. Therefore the length of the  $p$ -intervals (bandwidth) where the curve lies inside  $\mathcal{S}$  decreases. So, far from the resonance  $p_0$  the bandwidth is short,

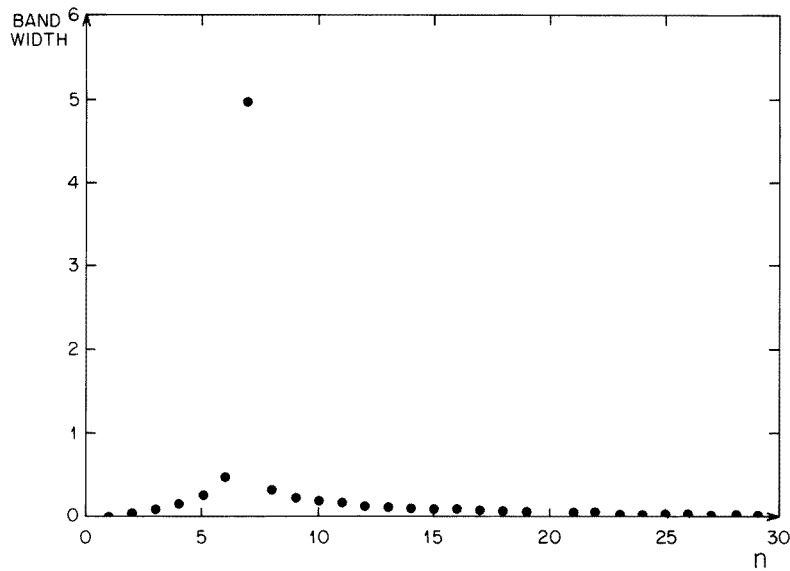


**Figure 3.** Plot of the function  $f(p)$  given by (5.3), which corresponds to a  $R(E)$  matrix with a single pole. Here  $p_0 = 7\pi$ , and  $\gamma_0^2 = \frac{1}{2}$ . The amplitude of the oscillations increases as  $p$  grows, except near  $p_0$  where the amplitude is small. The allowed values of  $p$  are those for which  $-1 \leq f(p) \leq 1$  as indicated in the text.



**Figure 4.** An amplification of figure 3. The almost vertical full lines between  $-1$  and  $1$  are the sections of the curve of figure 3 for which  $-1 \leq f(p) \leq 1$ . The dotted curves are the sections of that curve for which  $f(p)$  is outside of  $[-1, 1]$ . The allowed values of  $p$  are those for which  $-1 \leq f(p) \leq 1$ . These values are indicated as heavy lines on the horizontal axis.

but near  $p_0$  the bandwidth is larger as shown by the heavy lines on the horizontal axis in figure 4. In the limit  $p \rightarrow \infty$  the bandwidth tends to zero. This behaviour is very different from that corresponding to the Kronig–Penney model. Thus, transmission occurs mainly near the resonance, and not for all large energies. Indeed, for large energies, transmission occurs



**Figure 5.** The ordinates are the width of the bands of figure 4. The widest band is the one corresponding to the resonance.

only in very short bands whose length tends to zero. Figure 5 shows a plot of the bandwidth as a function of the band number  $n$ . As shown from comparing figures 4 and 5, the widest width of the band occurs when  $p_0$  is inside it.

5.3.  $R(E)$  function with one pole and one zero

The next case is when  $R(E)$  is given by two terms of (3.7):

$$R(E) = \frac{\gamma_0^2}{E_0 - E} + R_0. \tag{5.4}$$

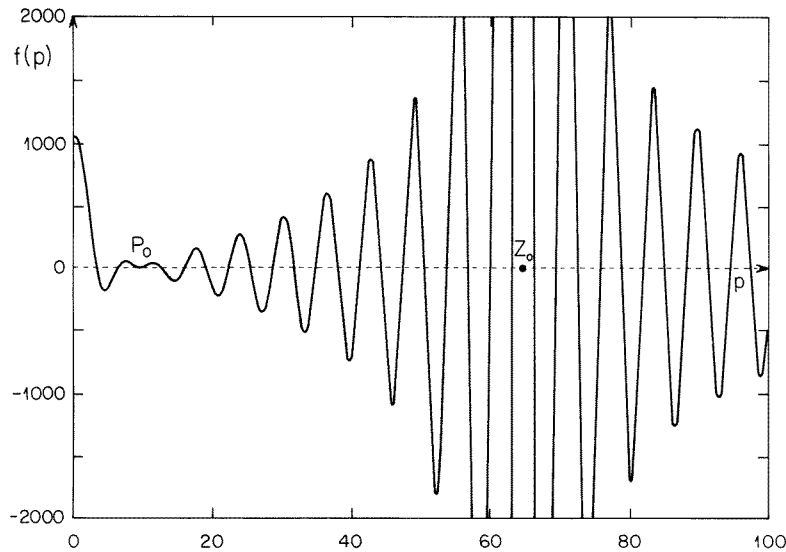
As we can see,  $R(E)$  has a single pole at  $E = E_0$  and a single zero at  $E = \frac{\gamma_0^2}{R_0} + E_0$ . Figure 6 shows a plot of

$$f(p) = \cos p + \frac{1}{\frac{4\gamma_0^2}{p_0^2 - p^2} + 2R_0} \frac{\text{sen } p}{p}. \tag{5.5}$$

The points  $p_0 = \sqrt{2E_0}$  and  $z_0 = \sqrt{2(\frac{\gamma_0^2}{R_0} + E_0)}$  are indicated in the figure where we can see their effects on the form of the curve. From the previous discussions (case 5.2) the behaviour of the pole at  $p_0$  is clear, so we will only discuss here the effect of the zero of  $R(p^2/2)$  at  $z_0$ . First, we note from (5.5) that for large  $p$ ,  $f(p)$  tends to  $\cos p$  as in the Kronig–Penney model. Thus, for large values of  $p$  the band structure will be very similar to that case. However, when  $p$  is near  $z_0$ , or equivalently, when  $E = \frac{\gamma_0^2}{R_0} + E_0 \pm \epsilon$  with  $\epsilon$  a small number, the factor  $\frac{1}{R(E)}$  suffers a very abrupt change. As a matter of fact,

$$R\left(\frac{\gamma_0^2}{R_0} + E_0 \pm \epsilon\right) = R_0 + \frac{\gamma_0^2}{E_0 - \frac{\gamma_0^2}{R_0} - E_0 \pm \epsilon} \approx R_0 \left(1 - \left(1_{\pm} \frac{\epsilon R_0}{\gamma_0^2}\right)\right) = \pm \frac{\epsilon R_0^2}{\gamma_0^2} \tag{5.6}$$





**Figure 6.** Plot of the function  $f(p)$  given by (5.5), which corresponds to a  $R(E)$  matrix with one pole and one zero. Here  $p_0 = 9.4$ ,  $\gamma_0^2 = 0.02$  and  $R_0 = 10^{-5}$ . The amplitude of the oscillations is small near the pole  $p_0$  and the amplitude exploits near the zero  $z_0$ . For large  $p$  the amplitude tends to 1.

which means that  $\frac{1}{R(E)}$  tends to  $+\infty$  at the left of  $z_0$  and to  $-\infty$  at the right. Thus, equation (4.12) has no solution for  $E = \frac{\gamma_0^2}{R_0} + E_0 = z_0^2/2$  as seen in figure 6. Near  $z_0$  the amplitude of the curve is large and therefore the bands around  $z_0$  are very thin.

Since at  $z_0$  the function  $R(E)$  is equal to zero, equation (3.6) implies that if  $\psi_{z_0}(x)$  was the corresponding wavefunction, then it would be equal to zero at the scattering centres. However, we have found that  $z_0$  is not a permitted value. Therefore  $\psi_{z_0}(x)$  is not a solution. This situation is the opposite of what is occurring in the Kronig–Penney model. In that case, if the wavefunction is zero at the delta potentials, the particles do not ‘feel’ the delta functions and the associated energy is a permitted value.

#### 5.4. $R(E)$ function of the picket-fence type

Our last example is a  $R(E)$  function with an infinite sequence of poles with the same residue, i.e.

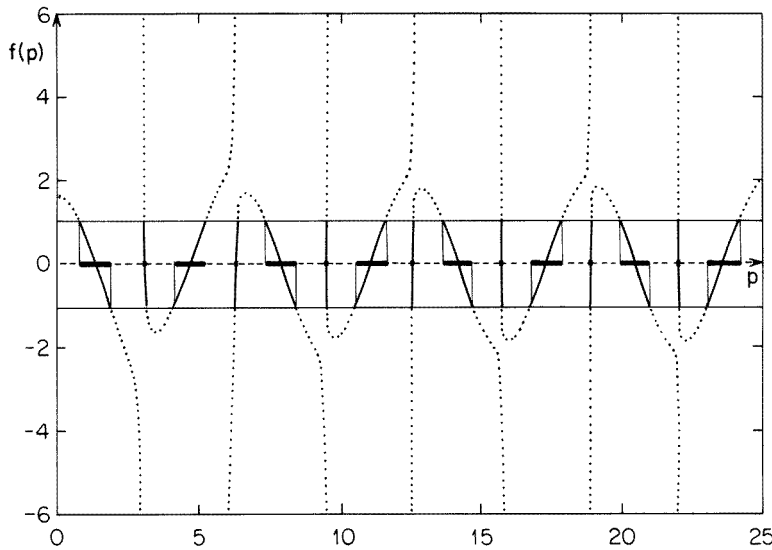
$$R(E) = \gamma^2 \sum_{n=1}^{\infty} \frac{1}{E_n - E} \quad (5.7)$$

where we choose  $E_n = \{[(n - \frac{1}{2})\pi]^2 - p_0^2\}/2$  with  $p_0$  being an arbitrary parameter. Now we use  $E = p^2/2$  and the identity [6]

$$\frac{\tan z}{z} = \sum_{n=1}^{\infty} \frac{2}{[(n - \frac{1}{2})\pi]^2 - z^2} \quad (5.8)$$

to write (5.7) as

$$R(E) = \gamma^2 \sum_{n=1}^{\infty} \frac{2}{[(n - \frac{1}{2})\pi]^2 - p_0^2 - p^2} = \gamma^2 \frac{\tan \sqrt{p^2 + p_0^2}}{\sqrt{p^2 + p_0^2}}. \quad (5.9)$$



**Figure 7.** Plot of the function  $f(p)$  given by (5.12), which corresponds to a  $R(E)$  matrix of the picket-fence type. Here  $p_0 = 1$ , and  $\gamma^2 = \frac{1}{2}$ . The bands are indicated as heavy lines on the horizontal axis.

Thus,

$$f(p) = \cos p + \frac{\sqrt{p^2 + p_0^2}}{2\gamma^2 \tan \sqrt{p^2 + p_0^2}} \frac{\text{sen } p}{p}. \tag{5.10}$$

Figure 7 shows a plot of this function which has an infinite number of poles and zeros, almost equally spaced in the momentum variable  $p$ . As in figure 4, the nearly vertical full lines between  $-1$  and  $1$  are the sections of the curve of  $f(p)$  for which  $-1 \leq f(p) \leq 1$ , giving the allowed bands which are also marked by heavy full lines on the abscissa. The dotted curves are the sections of that curve for which  $f(p)$  is outside of  $[-1, 1]$ . In this case the bands appear as couples. In each couple one band is wide and the other very thin.

Note that for  $p_0 = 0$  the values of  $p$  for which  $R(E) = 0$  are equally spaced and from (5.10)  $f(p) = [1 + 1/(2\gamma^2)] \cos p$  giving rise to a perfect picket fence. In this case all bands are identical and the permitted values of  $p$  inside each band are such that

$$-\frac{1}{1 + \frac{1}{2\gamma^2}} \leq \cos p \leq \frac{1}{1 + \frac{1}{2\gamma^2}}. \tag{5.11}$$

### 6. Conclusion

There is a fundamental difference between the passage of a beam of electrons or neutrons through a crystal. The electron interacts with the whole atom in the crystal whose dimensions are of the same order of magnitude as that of the interatomic distance.

The neutrons only interact with the nuclei through nuclear forces whose range is of the order  $10^{-12}$  cm, which is very small compared with the interatomic distance in the lattice, which is of the order of  $10^{-8}$  cm. Thus, one could make the approximation that the interactions of the neutrons take place at the *points* where the nuclei are present.

It would seem then that the *original* Kronig–Penney lattice with equally spaced delta function interactions would be a good one-dimensional model for the behaviour of the passage of neutrons through the lattice. This, however, does not take into account the structure of nuclei, and in particular, the resonant states. We have thus introduced in the one-dimensional model the  $\mathbf{R}$  matrix description of resonance nuclear theory given by Wigner [4, 5], with the internal region reduced to a point at the end of each segment of the lattice. The determination of the allowed bands can be obtained directly in a formula very similar to the one of Kronig–Penney but with an  $R$  function in the denominator of one of the terms.

We then discussed the behaviour of the allowed bands for particular cases of the  $R(E)$  function. When  $R(E)$  is just a constant we recover Kronig–Penney’s original result. When  $R(E)$  has a single pole, the wide allowed bands cluster around the resonance energy, or equivalently its corresponding momentum. Far away from the resonance the bands become isolated points and the change in the width of the bands in figure 5 clearly shows this behaviour; when  $R(E)$  has a pole and a zero, we see that for the former, the behaviour is similar to the one mentioned in the previous phrases, while for the latter the bands are very narrow in the vicinity of the energy for which  $R(E) = 0$ ; finally we discuss a kind of picket-fence form for  $R(E)$  and find that the allowed bands, alternatively wide and narrow, occur almost periodically through the whole range of momenta as shown in figure 7.

In the following appendix we discuss the single pole case with parameters taken from experiment.

### Acknowledgment

The authors would like to thank María Esther Ortiz for fruitful discussions.

### Appendix. Band structure for a neutron interacting with a one-dimensional crystal

In this appendix we will again discuss the case analysed in section (5.2) but now with realistic values for the parameters. We will take the values corresponding to a neutron  $n$  with mass  $m = 1.67 \times 10^{-24}$  g interacting with the nuclei of a one-dimensional chain of carbon atoms  $^{12}\text{C}$  with a lattice constant  $a = 3.56 \times 10^{-8}$  cm [2]. We will consider an energy of the incident neutron near to an isolated resonance in  $^{12}\text{C}(n, n)^{12}\text{C}$ , in such a way that the interaction can be described by means of an  $\mathbf{R}(E)$  matrix with a single resonance. In this case  $R(E)$  is given by (5.1), i.e.

$$R(E) = \frac{\gamma_0^2}{E_0 - E} \quad (\text{A.1})$$

where  $E_0$  and  $\gamma_0$  will be determined as follows. Since  $\mathbf{S} = (1 + i p \mathbf{R}(E))(1 - i p \mathbf{R}(E))^{-1}$  [3], with  $\mathbf{R}(E)$  having the form

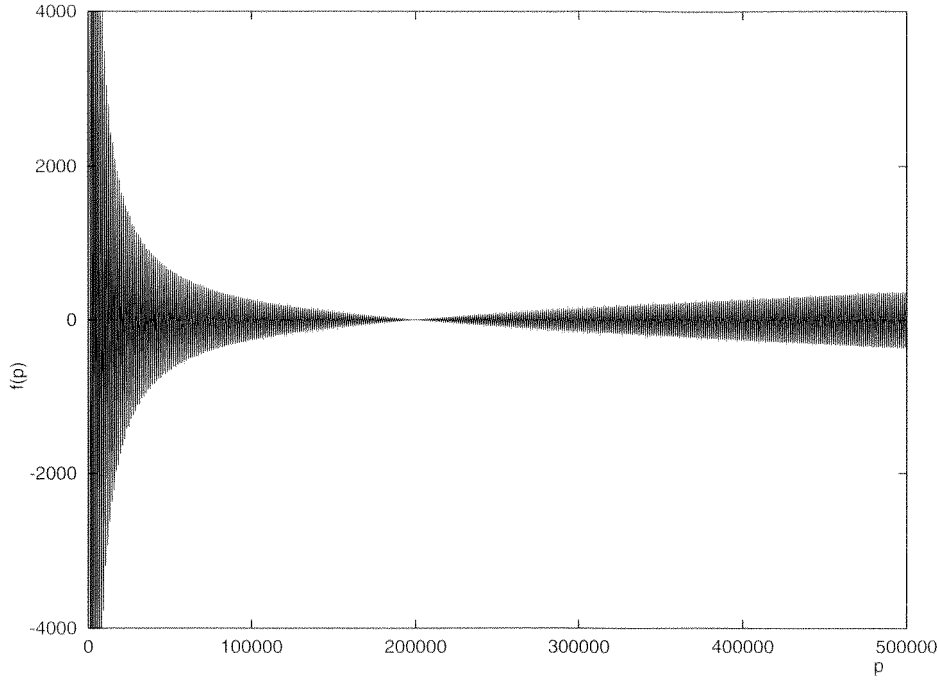
$$\mathbf{R}(E) = R(E) \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \quad (\text{A.2})$$

we obtain

$$\mathbf{S} = \begin{bmatrix} 1 & i2pR(E) \\ i2pR(E) & 1 \end{bmatrix} \frac{1}{1 - i2pR(E)}. \quad (\text{A.3})$$

Taking now for  $R(E)$  the form (5.1) and  $p_0^2 = 2E_0$ ,  $p^2 = 2E$  the  $\mathbf{S}$  matrix becomes

$$\mathbf{S} = \begin{bmatrix} p_0^2 - p^2 & i4p\gamma_0^2 \\ i4p\gamma_0^2 & p_0^2 - p^2 \end{bmatrix} \frac{1}{p_0^2 - p^2 - i4p\gamma_0^2} \quad (\text{A.4})$$



**Figure A1.** Same as in figure 3 ( $R(E)$  matrix with a single pole), but with the values of  $p_0$  and  $\gamma_0^2$  taken from the experiments. Here  $p_0 = \sqrt{2E_0} = 2.00 \times 10^5$ , and  $\gamma_0^2 = 282.31$ . In this case the  $p$ -interval analysed is large as compared with the period of the trigonometric functions. Thus, the oscillations appear very close. Near  $p_0$  there are many oscillations whose amplitude is of the order of 1. Therefore, there are many wide bands near  $p_0$  as seen in figure A2.

and therefore the pole in the right-hand side of the  $p$  complex plane is given by

$$\sqrt{p_0^2 - 4\gamma_0^4} - i2\gamma_0^2 \tag{A.5}$$

whose square divided by 2 is

$$(E_0 - 4\gamma_0^4) - i2\gamma_0^2\sqrt{2E_0 - 4\gamma_0^4}. \tag{A.6}$$

Now we identify the real and imaginary parts of this expression with the energy  $E_r$  and width  $\Gamma$  respectively of some particular resonance in  $^{12}\text{C}(n, n)^{12}\text{C}$ . Thus, we have

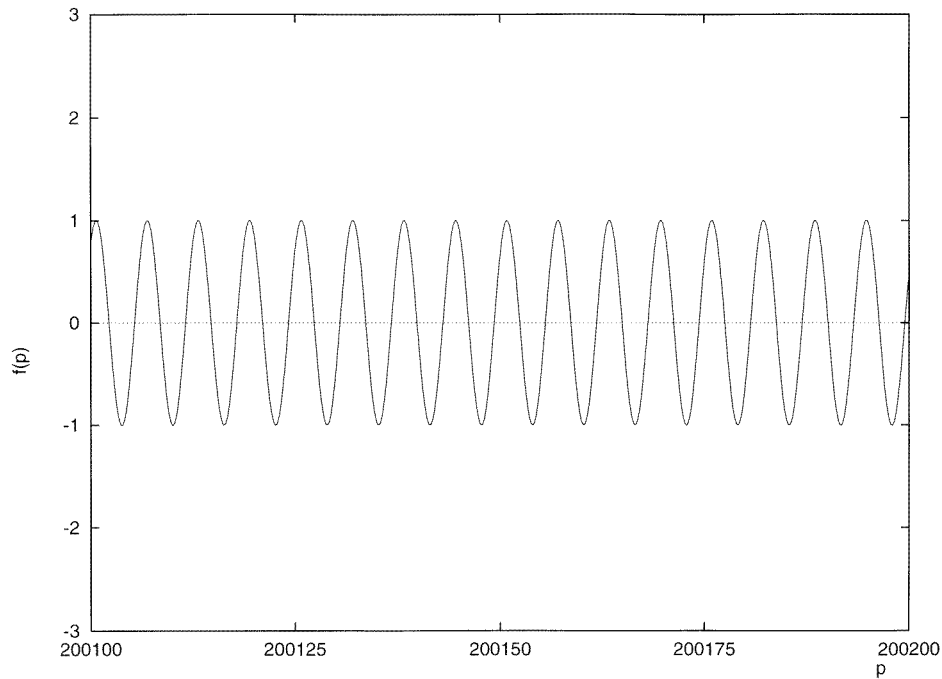
$$E_0 = \sqrt{E_r^2 + \Gamma^2} \tag{A.7}$$

and

$$4\gamma_0^4 = \sqrt{E_r^2 + \Gamma^2} - E_r. \tag{A.8}$$

The chosen resonance is  $E_r = 6.558$  MeV with  $\Gamma = 37$  Kev which is a reasonably isolated resonance corresponding to a channel with  $l = 0$  [7]. In our units ( $\hbar = m = a = 1$ ) these values become  $E_r = 2.003 \times 10^{10}$  and  $\Gamma = 1.13 \times 10^8$ . Therefore, since  $E_r \gg \Gamma$ , we have  $E_0 = E_r = 2.003 \times 10^{10}$  and  $\gamma_0^2 = \frac{\Gamma}{\sqrt{8E_r}} = 282.31$ .

Figure A1 shows a plot of  $f(p)$  with  $R(E)$  given by (A.1) with the values of  $E_0$  and  $\gamma_0^2$  as calculated above. In this case  $p_0 \gg 2\pi$  and consequently there are very many oscillations of  $f(p)$  between  $p = 0$  and  $p = p_0$ . Furthermore, far away from  $p_0$  the amplitude of the



**Figure A2.** We amplify the part of figure A1 that is close to  $p_0$ .

oscillations is large and therefore the width of the bands are very small. However, near  $p_0$ , there are also many oscillations but now with small amplitude as shown in figure A2. Thus, near  $p_0$  there are many bands with wide width. So, transmission occurs near  $p_0$  but in many bands and not only in a single band as in the case of figure 4. Indeed, near  $p_0$ , there are a large number of bands separated by small gaps.

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