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Scattering states for a finite chain in one dimension

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Abstract. Using the transfer matrix method, the solution of the scattering problem on the finite periodic chain of equal symmetric potentials is found in terms of the partial reflection and transmission coefficients. A simple algebraic result is presented showing that the transmission coefficient oscillates rapidly between one and some lower value when the energies lie in the allowed Bloch band. A special case of δ potentials is discussed using the momentum representation. The explicit form for the transmission amplitude can also be used to determine positions of the bound states.

1. Introduction

Since the historic paper of Kronig and Penney (1930) on electron motion in an infinite or half-infinite one-dimensional periodic chain of δ potentials, this model has served as a valuable tool in explaining several interesting physical properties of real materials. It is surprising, however, that the corresponding problem with a finite number of scattering centres does not seem, at least to our knowledge, to have merited comparable attention. Pshenichnov (1962) has investigated the scattering problem on a periodic finite chain of identical potentials using the WKB approximation and has shown the existence of a resonance effect in the transmission coefficient. Reading and Siegel (1972) have considered particle scattering from a finite chain of δ potentials of arbitrary strengths and positions, using the momentum representation.

The aim of this article is to present an exact solution of the scattering problem for a finite chain of N equally-spaced symmetric potentials. Using the transfer matrix method one can derive a simple algebraic expression for the total transmission coefficient (§ 2) containing two parameters of the partial reflection and transmission coefficients by which a single potential, forming a chain, is characterised. The resonance effects are observed when the transmission coefficient is exactly equal to one. The corresponding energies lie in the allowed Bloch bands of an infinite periodic chain. It seems that the latter property is valid only for the strictly periodic structure. The general results are also illustrated for a δ potential model (§ 3), using the momentum representation.

2. Scattering states via the transfer matrix method

One considers the scattering of one particle off a finite one dimensional chain of equally-spaced identical potentials $v(x)$. The total potential takes the form

$$U(x)=\sum_{j=0}^{N-1} v(x-ja) \tag{1}$$

where $v(x)$ is a symmetric potential, $v(x)=v(-x)$, which vanishes outside of the interval $-\frac{1}{2}a<x<\frac{1}{2}a$. In what follows the units $\hbar=2m=a=1$ are adopted.

The wavefunction can be written in the form

$$\psi(x)=\exp(\mathrm{i}Kx)+R\exp(-\mathrm{i}Kx), \qquad x<-\tfrac{1}{2} \tag{2}$$

$$\psi(x)=a_j\{t\exp[\mathrm{i}K(x-j)]\}+b_j\{\exp[-\mathrm{i}K(x-j)]+r\exp[\mathrm{i}K(x-j)]\}, \qquad x\sim j+\tfrac{1}{2} \tag{3a}$$

$$\psi(x)=a_j\{\exp[\mathrm{i}K(x-j)]+r\exp[-\mathrm{i}K(x-j)]\}+b_j\{t\exp[-\mathrm{i}K(x-j)]\}, \qquad x\sim j-\tfrac{1}{2} \tag{3b}$$

$$\psi(x)=T\exp\mathrm{i}Kx, \qquad x>N-\tfrac{1}{2}. \tag{4}$$

Equations (2) and (4) define the reflection and transmission amplitudes. The validity of the forms (3a) and (3b) is restricted to the region where the potential (1) is zero. They represent a linear combination of the two independent wavefunctions for scattering from a single symmetric potential $v(x)$, with incident waves coming from opposite directions (Ashcroft and Mermin 1976). The asymptotic forms contain the partial energy-dependent reflection and transmission amplitudes, r and t respectively. The transfer matrix $\mathbf{M}$ (Hori 1968)

$$\begin{pmatrix} a_{j-1} \\ b_{j-1} \end{pmatrix}=\mathbf{M}\begin{pmatrix} a_j \\ b_j \end{pmatrix} \tag{5}$$

is determined by requiring the equality of the wavefunctions (3a) and (3b) and their derivatives at the point $x=j-\frac{1}{2}$:

$$\mathbf{M}=\begin{pmatrix} t\exp(\mathrm{i}K) & r\exp(\mathrm{i}K) \\ -r\exp(\mathrm{i}K) & \dfrac{\exp(-\mathrm{i}K)-r^2\exp(\mathrm{i}K)}{t} \end{pmatrix}. \tag{6}$$

Finally

$$\begin{pmatrix} a_{N-1} \\ b_{N-1} \end{pmatrix}=\mathbf{M}^{-(N-1)}\begin{pmatrix} a_0 \\ b_0 \end{pmatrix} \tag{7}$$

together with the boundary conditions

$$ta_{N-1}=T \qquad b_{N-1}=0 \tag{8a}$$

$$ta_0=1-rR \qquad b_0=R. \tag{8b}$$

The matrix $\mathbf{M}^{-(N-1)}$ is evaluated by the Lagrange–Sylvester formula:

$$f(\mathbf{M})=f(\lambda_1)\frac{\lambda_2-\mathbf{M}}{\lambda_2-\lambda_1}+f(\lambda_2)\frac{\lambda_1-\mathbf{M}}{\lambda_1-\lambda_2}. \tag{9}$$

The parameters λ_1 and λ_2 are the eigenvalues of the matrix $\mathbf{M}$:

$$\lambda_1=\exp(\mathrm{i}k) \qquad \lambda_2=\exp(-\mathrm{i}k) \tag{10}$$

where the wavevector k is expressed through r and t:

$$\cos k=\tfrac{1}{2}\left(\frac{t^2-r^2}{t}\exp(\mathrm{i}K)+\frac{1}{t}\exp(-\mathrm{i}K)\right)=\frac{\cos(K+\delta)}{|t|} \tag{11}$$

with

$$t=|t|\exp\mathrm{i}\delta \qquad r=\mathrm{i}|r|\exp\mathrm{i}\delta \qquad |t|^2+|r|^2=1. \tag{12}$$

Hence the matrix $\mathbf{M}^{-(N-1)}$ is expressed in the form

$$\mathbf{M}^{-(N-1)} = \begin{pmatrix} \dfrac{\sin Nk}{\sin k} - t\exp(\mathrm{i}K)\dfrac{\sin(N-1)k}{\sin k} & -r\exp(\mathrm{i}K)\dfrac{\sin(N-1)k}{\sin k} \\ r\exp(\mathrm{i}K)\dfrac{\sin(N-1)k}{\sin k} & \dfrac{\sin Nk}{\sin k} - \dfrac{\exp(-\mathrm{i}K) - r^2\exp(\mathrm{i}K)}{t}\dfrac{\sin(N-1)k}{\sin k} \end{pmatrix}. \tag{13}$$

The final expressions for the transmission amplitude T and the transmission coefficient $|T|^2$ are

$$T = \frac{\exp[-\mathrm{i}(N+1)K]}{\cos Nk - \mathrm{i}(\sin(K+\delta)/|t|)(\sin Nk/\sin k)}, \tag{14}$$

$$|T|^2 = \frac{1}{1 + |r/t|^2(\sin^2 Nk/\sin^2 k)}. \tag{15}$$

The wavevector k defined through equation (11) can be either real or pure imaginary, according as $|\cos k|$ is less than or greater than one. This corresponds to the usual distinction between the allowed and forbidden energy bands of an infinite chain. From the form (15) one can see the typical oscillatory behaviour of the transmission coefficient in the allowed bands, reaching the value one exactly at $N-1$ points when $k = nj\pi/N$, with n labeling the particular band and j running between $1 \leq j \leq N-1$. With increasing negative strength of the potential (1) the number of energies in the first energy band with $|T|^2 = 1$ gradually diminishes. In the forbidden bands the transmission coefficient (15) is always less than one.

3. Scattering states illustrated by a δ potential model

When the potential is formed by a chain of δ functions $U(x) = V\Sigma_{j=0}^{N-1}\delta(x-j)$, a convenient method leading to the solution (15) is also furnished by considering the Schrödinger equation in the momentum representation:

$$(q^2 - K^2)\phi(q) + \frac{V}{2\pi}\sum_{j=0}^{N-1}\left(\exp(-\mathrm{i}qj)\int_{-\infty}^{+\infty}\exp(\mathrm{i}q'j)\phi(q')\,\mathrm{d}q'\right) = 0. \tag{16}$$

The solution $\phi(q)$ containing only outgoing scattered waves has the form

$$\phi(q) = \frac{\Sigma_{j=0}^{N-1}\exp(-\mathrm{i}qj)c_j}{\pi(q^2 - K^2 - \mathrm{i}\epsilon)} + \delta(q-K) \tag{17}$$

or in coordinate space:

$$\psi(x) = \exp(\mathrm{i}Kx) + \frac{\mathrm{i}}{K}\sum_{j=0}^{N-1} c_j\exp(\mathrm{i}K|x-j|). \tag{18}$$

The amplitudes of the scattered waves satisfy the set of linear inhomogeneous equations

$$-\frac{\mathrm{i}K}{V}c_n + \sum_{j=0}^{N-1}\exp(\mathrm{i}K|x-j|)c_j = \mathrm{i}K\exp(\mathrm{i}Kn), \qquad n = 0, 1, \ldots, N-1 \tag{19}$$

which can be cast in the form

$$\left(2\sin K+\frac{K}{V}\exp(-\mathrm{i}K)\right)c_0-\frac{K}{V}c_1=2\mathrm{i}K\sin K \qquad (20a)$$

$$\frac{K}{V}c_{N-2}-\left(2\sin K+\frac{K}{V}\exp(-\mathrm{i}K)\right)c_{N-1}=0 \qquad (20b)$$

$$c_{j+2}-2\cos k c_{j+1}+c_j=0, \qquad j=0,1,\ldots,N-3 \qquad (20c)$$

where

$$\cos k=\cos K+\frac{V}{K}\sin K. \qquad (21)$$

The equivalence of the two sets (19) and (20) of equations can be directly verified by adding respectively the first and second rows, the $(N-1)$th and the Nth rows, as well as the jth and the $(j+2)$th rows of the set (19), multiplied by suitable factors.

The set (20c) leads to the solution

$$c_n=\gamma_1\exp(\mathrm{i}kn)+\gamma_2\exp(-\mathrm{i}kn) \qquad (22)$$

where the two constants γ_1 and γ_2 are determined through (20a) and (20b). Finally from the wavefunction (18) the results (14) and (15) for the transmission amplitude and coefficient are easily reproduced:

$$T=\frac{\exp[-\mathrm{i}(N+1)K]}{\cos Nk-\mathrm{i}[(V/K)\sin K-\cos K]\sin Nk/\sin k}, \qquad (23)$$

$$|T|^2=\frac{1}{1+(V/K)^2(\sin^2 Nk/\sin^2 k)}. \qquad (24)$$

Equation (16) can also be used for the calculation of the energy levels of the bound states. According to general principles they are identified as the poles of the transmission amplitude T lying on the imaginary axis of the K plane (Newton 1966). One can see that the number of bound states is equal to N when $|\cos k|<1$. They begin to disappear in the region $-2<V<0$, where the number of missing states is equal to the integer part of $(N/\pi)\cos^{-1}(-1-V)$.

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