The Scattering Matrix Method in the Linear Chain

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§1. Introduction

The method of scattering-matrix (S-matrix) was first applied to the problem of vibration of imperfect chains by Y. Fukuda.\textsuperscript{13} The merit of this method lies in that the aspect of the vibration can be vividly visualized. It is especially useful for treating the localized mode, owing to the fact that its frequency is given by the pole of S-matrix. When there are several impurities, however, the direct application of the S-matrix method leads to involved calculations. In this article, a systematic method is presented, which is based upon the algebra of S-matrices effectively used by Redheffer\textsuperscript{3} in his transmission-line theory, and makes it possible to cope with the problem of several impurities with only a reasonable amount of calculations.

As a preparation, the S-matrix associated with an individual impurity is calculated in §2 by the ordinary method. The algebra of S-matrices is introduced in §3. It is shown that a localized mode can be considered as the wave which happens to enter between two impurities—two partly reflective walls—, and continues to ply between two impurities and cannot escape from that region.

As an illustration of our method, some simple problems are considered in §4. The stress is laid on the localized-mode problem, but it is also shown that it is possible to treat the ordinary normal mode as if it were a localized mode trapped between two boundaries. It is also seen that the localized mode associated with the impurities at the free boundary can be understood as that trapped between the boundary and the impurities.

§2. The definition of the scattering matrix of an isotopic impurity

We consider a chain of infinite number of atoms whose masses are all equal to $M$, except for a mass $M'$ of an isotopic impurity located at lattice site $n$. All atoms are coupled to its nearest neighbors by elastic springs which obey Hooke’s law and have the same elastic modulus $\gamma$. Only the longitudinal vibrations of the chain are studied. Then the equations of motion of the chain are

$$M\ddot{x}_j = \gamma(x_{j+1} - 2x_j + x_{j-1}), \text{ for } j \neq n,$$
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\[ M' \dot{x}_n = r (x_{n+1} - 2x_n + x_{n-1}), \]

where \( x_j \) is the displacement of the atom at lattice site \( j \) from its equilibrium position.

To construct the S-matrix of the isotopic impurity, we discuss the scattering of plane wave by the isotopic impurity. Except at the isotopic impurity, a plane wave

\[ x_j = A \exp \{i (j \varphi - \omega t) \}, \]

where \( \omega = \omega_L \sin (\varphi/2) \), \( \omega_L = \sqrt{4r/M} \), can propagate through the lattice. However, because of the scattering of the plane wave by the isotopic impurity, the total displacement of the \( j \)-th atom is the sum of the incident plane wave and a scattered wave:

\[ x_j = Ae^{-iat} u(j), \]

where

\[ v(j) = u(j) + e^{i\varphi}. \]

The scattered wave \( u(j) \) is the solution of the equations

\[ Lu(j) = M \omega^2 u(j) + r[u(j+1) - 2u(j) + u(j-1)] = (M - M') \omega^2 [u(j) + e^{i\varphi}] \delta_{j, \ast}, \]

where \( \delta_{j, \ast} \) is Kronecker's delta. The general solution of the above equation can be represented in terms of the Green's function \( g(j) \) as

\[ u(j) = 4f^3(1-Q)g(j-n) [u(n) + e^{i\varphi}], \]

where \( f^2 = (\omega/\omega_L)^2 \), \( Q = M'/M \) and the Green's function is defined by

\[ Lg(j) = 7g_{j,0}. \]

By setting \( j = n \), \( u(n) \) is found to be

\[ u(n) = \frac{4f^3(1-Q)g(0)}{1 - 4f^3(1-Q)g(0)} e^{i\varphi} = \frac{a}{1-a} e^{i\varphi}, \]

\[ a = 4f^3(1-Q)g(0). \]

To complete the expression of the scattered wave, the Green's function \( g(j) \) must be specified. The Fourier transform \( g(\phi) \) of \( g(j) \) defined by

\[ g(j) = \frac{1}{2\pi} \int_{-\pi}^{\pi} g(\phi) e^{ij\phi} d\phi, \]

is easily found to be

\[ g(\phi) = \frac{1}{2} \frac{1}{\cos \phi - \cos \varphi}. \]
The Green’s function $g(j)$ is then given by

$$g(j) = \frac{1}{4\pi} \int_{-\pi}^{+\pi} \frac{e^{i\phi} - \cos \phi}{\sin \phi} d\phi = \frac{1}{2\pi i} \oint_C \frac{z^j}{(z - e^{i\varphi})(z - e^{-i\varphi})} dz.$$ 

Here the path $C$ is chosen to be a unit circle with a counter-clock wise sense, including only a pole at $e^{i\varphi}$. Thus $g(j)$ is found to be

$$g(j) = \frac{e^{i|j|\varphi}}{2i \sin \varphi},$$

and the total displacement becomes

$$u(j) = e^{i\varphi} + \frac{a}{1-a} e^{i\varphi}, \quad j \geq n$$

$$= e^{i\varphi} + \frac{ae^{2i\varphi}}{1-a} e^{-i\varphi}, \quad j \leq n.$$

We consider the incoming part of the vibration of the $(n-1)$-th atom as the input to the $n$-th atom from left, and the outgoing part of the vibration of the $(n-1)$-th atom as the wave reflected at the $n$-th atom, or the output to left from the $n$-th atom (left-hand reflection). Moreover the outgoing part of the vibration of the $n$-th atom is considered as the transmitted part of the input from left to the $n$-th atom or the output to right from the $n$-th atom (left-hand transmission). Then the left-hand transmission coefficient of the $n$-th atom is defined as

$$t = \frac{1}{1-a} e^{in\varphi} = \frac{e^{i\varphi}}{1-a},$$

and the left-hand reflection coefficient of the $n$-th atom is defined as

$$r = \frac{ae^{2in\varphi}}{e^{i(n-1)\varphi} - 1-a} = \frac{a}{1-a} e^{2i\varphi}.$$

Similarly if we have a plane wave travelling from right to left, and we consider the direction of the incident wave as incoming and the opposite direction as outgoing direction, the input from right to the $n$-th atom and the output to right from the $n$-th atom are defined as the incoming part and the outgoing part of the vibration of the $n$-th atom, respectively. Further, an outgoing vibration of the $(n-1)$-th atom is defined as an output to left from the $n$-th atom. Then the right-hand transmission coefficient and the right-hand reflection coefficient of the $n$-th atom are found to be

$$\tau = \frac{e^{i\varphi}}{1-a}.$$
and

$$\rho = \frac{a}{1-a},$$

respectively.

As a result, we get the S-matrix of the isotopic impurity as

$$\begin{pmatrix} t & \rho \\ r & \tau \end{pmatrix} = \begin{pmatrix} e^{i\rho} & a \\ \frac{a e^{i\tau}}{1-a} & e^{i\tau} \end{pmatrix}.$$ 

Also the S-matrix of a host atom is easily found to be

$$\begin{pmatrix} e^{i\rho} & 0 \\ 0 & e^{i\rho} \end{pmatrix},$$

by setting $a=0$.

§3. Algebra of the scattering matrix

An element is defined as consisting of an atom and a spring attached to it on its left-hand side like a tail. (See Fig. 1.) The elements are joined one after another in a straight line to form a chain. In Fig. 1 an element specified by the S-matrix $(t, \tau, r, \rho)$ is taken out from the chain, where complex numbers $z_i$ represent amplitudes of waves propagating as shown, so that odd subscripts refer to the propagation from left to right and even subscripts to that from right to left. The principle of superposition combined with the definition of $t, \tau, r$ and $\rho$ yields

$$\begin{pmatrix} z_3 \\ z_2 \end{pmatrix} = \begin{pmatrix} t & \rho \\ r & \tau \end{pmatrix} \begin{pmatrix} z_1 \\ z_4 \end{pmatrix}.$$ 

Let an element with coefficients $(t, \tau, r, \rho)$ be placed adjacent to the second element having coefficients $(t_1, \tau_1, r_1, \rho_1)$ as shown in Fig. 2. Besides the relation connecting $(z_1, z_4)$ and $(z_3, z_2)$, the following relation exists;

$$\begin{pmatrix} z_3 \\ z_2 \end{pmatrix} = \begin{pmatrix} t_1 & \rho_1 \\ r_1 & \tau_1 \end{pmatrix} \begin{pmatrix} z_1 \\ z_0 \end{pmatrix}.$$ 

On solving for $z_3$ and $z_2$ in terms of $z_1$ and $z_0$, we get
\[
\begin{pmatrix}
  z_5 \\
  z_2 \\
\end{pmatrix} = \begin{pmatrix}
  t_1 (1 - \rho r_1)^{-1} t & \rho_1 + t_1 \rho (1 - r_1 \rho)^{-1} \tau_1 \\
  r + \tau r_1 (1 - \rho r_1)^{-1} t & \tau (1 - r_1 \rho)^{-1} \tau_1 \\
\end{pmatrix} \begin{pmatrix}
  z_1 \\
  z_6 \\
\end{pmatrix}.
\]

This matrix is the S-matrix for the composite system consisting of the first element immediately followed by the second. This associated linear transformation is denoted as the star product
\[
\begin{pmatrix}
  t & \rho \\
  r & \tau \\
\end{pmatrix}^* \begin{pmatrix}
  t_1 & \rho_1 \\
  r_1 & \tau_1 \\
\end{pmatrix}.
\]

The star multiplication is easily seen to be associative i.e., that
\[
S_1^* (S_2^* S_3) = (S_1^* S_2) S_3,
\]
for 2 by 2 complex matrices \(S_i\). A physical interpretation of star product will prove useful for further development. If the incident wave has the unit amplitude, then the complex amplitude of the wave moving from left to right between the adjacent atoms is
\[
A = t (1 + r_1 \rho + (r_1 \rho)^2 + (r_1 \rho)^3 + \cdots) = \frac{t}{1 - r_1 \rho},
\]
provided \(|r_1 \rho| < 1\). The factor \((1 - r_1 \rho)^{-1}\) represents a measure of the ability of trapping the wave between the two adjacent atoms which happens to enter in this region. We shall see that the case in which this factor becomes infinite, in other words \(\rho r_1 = 1\), corresponds to the occurrence of a localized mode. Now let this resultant wave \(A\) proceed through the second element, then the left-hand transmission coefficient is obtained as
\[
\frac{t}{1 - r_1 \rho} t_1.
\]

Similarly, letting the wave \(A\) be reflected at the second element and transmit from right to left through the first, we have
\[
r + \frac{t}{1 - r_1 \rho} r_1 \tau,
\]
as the left-hand reflection coefficient.

The S-matrix for a series of identical elements which consists of some host atoms and isotopes can be obtained by a continued star product. The star-product preserves the property \(t = \tau\). First let us consider the condition that two S-matrices commute with each other, i.e. they give the same result independently of their order in the chain. The equation
\[
\begin{pmatrix}
  t & \rho \\
  r & \tau \\
\end{pmatrix}^* \begin{pmatrix}
  t_1 & \rho_1 \\
  r_1 & \tau_1 \\
\end{pmatrix} = \begin{pmatrix}
  t_1 & \rho_1 \\
  r_1 & \tau_1 \\
\end{pmatrix}^* \begin{pmatrix}
  t & \rho \\
  r & \tau \\
\end{pmatrix},
\]
is equivalent to
\[ \frac{r}{\rho} = \frac{r_1}{\rho_1}, \]

together with
\[ \frac{t \tau - \rho r - 1}{2 \rho} = \frac{t_1 \tau_1 - \rho_1 r_1 - 1}{2 \rho_1}. \]

If we define the two ratios
\[ A = \frac{r}{\rho}, \quad B = \frac{t \tau - \rho r - 1}{2 \rho}, \]

the necessary and sufficient condition of the commutability of S-matrices is that both S-matrices have the same A and B. In case the element specified by \( t, t, r \) and \( \rho \) is repeated \( n \) times, the over-all scattering matrix is given by
\[ \begin{pmatrix} t_* & \rho_* \\ r_* & t_* \end{pmatrix} = \begin{pmatrix} t & \rho \\ r & t \end{pmatrix}^n, \]
in the sense of star product. Since identical elements commute with each other, we can express \( t_* \) and \( r_* \) in terms of \( \rho_* \), namely.
\[ r_* = A \rho_*, \]
\[ t_* = 1 + 2B \rho_* + A \rho_*^2. \]

What remains to be done is to get the expression for \( \rho_* \). This can be obtained by solving the difference equation
\[ \rho_{n+1} = \rho + \frac{t^2}{1 - r \rho_*} \rho_* . \]

The solution of this equation is given in Appendix B. The result is
\[ \rho_* = \frac{\rho \sinh(n \delta)}{\sinh(n \delta) - t \sinh(n-1) \delta}, \]
\[ t_* = \frac{t \sinh \delta}{\sinh(n \delta) - t \sinh(n-1) \delta}, \]

where \( \delta \) is defined by
\[ 2t \cosh \delta = 1 + t^2 - \rho r. \]

The expression for \( r_* \) is obtained by merely exchanging \( r \) with \( \rho \).

It is convenient to represent the boundary conditions in the form of S-matrix. By the aid of the S-matrix of the boundaries, the normal modes of a finite chain can be treated as localized modes trapped between two
boundaries. Also the effect of end impurities can be treated as a problem of the localized mode trapped between a free boundary and isotopic impurities.

Setting \( a=\infty \) in the S-matrix of the isotopic impurity, the S-matrix of the rigid boundary is easily obtained as

\[
\left( \begin{array}{cc} 0 & -1 \\ -e^{i\varphi} & 0 \end{array} \right).
\]

This matrix can be rewritten as

\[
\left( \begin{array}{cc} e^{i\varphi} & 0 \\ 0 & e^{i\varphi} \end{array} \right)^* \left( \begin{array}{cc} 0 & -1 \\ -1 & 0 \end{array} \right).
\]

Thus it is seen that the rigid boundary consists of two operations; one is the operation of advancing phase by an amount \( \varphi \) and the other is a perfect reflection with phase change \( \pi \).

As the result of the above consideration, the S-matrix of the free boundary can be inferred to be the product of an operation of advancing the phase by \( \varphi/2 \) and an operation of perfect reflection without any phase change. If the right end is free, the S-matrix of the free boundary is found to be

\[
\left( \begin{array}{cc} e^{i(\varphi/2)} & 0 \\ 0 & e^{i(\varphi/2)} \end{array} \right)^* \left( \begin{array}{cc} 0 & 1 \\ 1 & 0 \end{array} \right) = \left( \begin{array}{cc} 0 & 1 \\ e^{i\varphi} & 0 \end{array} \right),
\]

and for the case the left end is free, the S-matrix has the form

\[
\left( \begin{array}{cc} 0 & 1 \\ 1 & 0 \end{array} \right)^* \left( \begin{array}{cc} e^{-i(\varphi/2)} & 0 \\ 0 & e^{-i(\varphi/2)} \end{array} \right) = \left( \begin{array}{cc} 0 & e^{-i\varphi} \\ 1 & 0 \end{array} \right).
\]

\section*{4. Impurity levels}

1) \textit{One impurity problem}

a) The case without the influence of the boundary\(^9\).

In this case, \( a=1 \) is the condition which leads to the divergence of the S-matrix. Setting \( \varphi=\pi+iz \), the above condition becomes

\[
(1-Q) \coth \frac{z}{2} = 1,
\]

which determines the value of \( z \) corresponding to a localized mode. Solving the above equation, the value of \( z \) which corresponds to the localized mode is obtained as
The frequency of the localized mode is determined by the dispersion relation

\[ \omega^2 = \omega_L \frac{1 + \cos x}{2}. \]

b) Localized modes trapped between an isotopic impurity and a boundary\(^{\text{pp}}\)

Let an isotopic impurity be located at the distance of \((n-1)\) host atoms from the rigid boundary, as shown in Fig. 3. This chain is represented by the S-matrix product:

\[
\begin{pmatrix}
\frac{e^{i\varphi}}{1-a} & \frac{a}{1-a} \\
\frac{ae^{i\varphi}}{1-a} & \frac{e^{i\varphi}}{1-a}
\end{pmatrix}
\times
\begin{pmatrix}
{e^{i(n-1)\varphi}} & 0 \\
0 & {e^{i(n-1)\varphi}}
\end{pmatrix}
\times
\begin{pmatrix}
0 & -1 \\
-e^{2i\varphi} & 0
\end{pmatrix}.
\]

On performing star products, the propagator between the isotopic impurity and the rigid boundary is found to be

\[
\left(1 + \frac{a}{1-a}e^{2i\varphi}\right)^{-1}.
\]

If we put \(\varphi = \pi + 2iz\), the value of \(z\) which leads to the divergence of the propagator is determined by

\[ a = \frac{1}{1-e^{2inz}}, \quad \text{where} \quad a = (1-Q) \coth\left(\frac{z}{2}\right). \]

In case an isotopic impurity is located at the distance of \((n-1)\) host atoms from the free boundary, as shown in Fig. 4, the S-matrix product from which the propagator between the isotopic impurity and the free boundary is calculated is found to be

\[
\begin{pmatrix}
\frac{e^{i\varphi}}{1-a} & \frac{a}{1-a} \\
\frac{ae^{i\varphi}}{1-a} & \frac{e^{i\varphi}}{1-a}
\end{pmatrix}
\times
\begin{pmatrix}
{e^{i(n-1)\varphi}} & 0 \\
0 & {e^{i(n-1)\varphi}}
\end{pmatrix}
\times
\begin{pmatrix}
0 & 1 \\
{e^{2i\varphi}} & 0
\end{pmatrix}.
\]
If we set $\varphi = \pi + iz$, the value of $z$ which gives a localized mode is determined by
\[ a = \frac{1}{1 - e^{-(a-1)x}}, \quad \text{where} \quad a = (1 - Q) \coth \left( \frac{x}{2} \right). \]

By putting $n = 1$, the value of $z$ corresponding to the localized mode due to an end impurity is found to be
\[ z = \log \left( \frac{1 - Q}{Q} \right). \]

c) Localized modes trapped between two boundaries

Normal modes$^p$.

From the viewpoint of S-matrix method, we must make a wave propagate to a scatterer from a distant point and deduce the characteristics of the scatterer by observing the tail of scattered wave again at a distant point. In the case of normal modes, any wave can not emerge from the boundaries, so we cannot observe the tail. Thus we must take a new standpoint, that is, we observe a wave at the inside of two boundaries. As an example of this method, we only consider the case in which one isotopic impurity is contained in our chain whose ends are fixed rigidly as shown in Fig. 5.

\[ \begin{array}{cccccccc}
  & & & & & & & \\
  & & & & & & & \\
  & & & & & & & \\
  & & & & & & & \\
  & & & & & & & \\
  & & & & & & & \\
 \end{array} \]

Fig. 5.

The S-matrix corresponding to the above chain is written as
\[
\begin{pmatrix}
  0 & -1 \\
  -e^{zi\varphi} & 0
\end{pmatrix}
\begin{pmatrix}
  e^{iz\varphi} & 0 \\
  0 & e^{iz\varphi}
\end{pmatrix}
\begin{pmatrix}
  e^{iz\varphi} & a \\
  1-a & 1-a
\end{pmatrix}
\begin{pmatrix}
  e^{iz\varphi} & 0 \\
  0 & e^{iz\varphi}
\end{pmatrix}
\begin{pmatrix}
  0 & -1 \\
  -e^{zi\varphi} & 0
\end{pmatrix}.
\]

On performing star products of four S-matrix except for the left-most S-matrix, it becomes
\[
\begin{pmatrix}
  0 & -1 \\
  -e^{zi\varphi} & 0
\end{pmatrix}
\begin{pmatrix}
  a e^{zi(N+n)\varphi} \\
  1-a
\end{pmatrix}
\begin{pmatrix}
  \left( e^{ziN\varphi} \right)^2 \\
  1 + a e^{zi(N-n)\varphi}
\end{pmatrix}^{-1},
\]
where the blank entries are irrelevant. The inverse of the propogator of the system comes out to be
\[ 1 + \frac{a e^{zi(N+n)\varphi}}{1-a} \left( \frac{e^{ziN\varphi}}{1-a} \right)^2 \left( 1 + \frac{a}{1-a} e^{zi(N-n)\varphi} \right)^{-1}. \]
After some straightforward calculations, we get the following equation which determines the values of $z$ making the above expression zero:

$$\sin(N\phi) \cdot \cos(N\phi) = (Q-1) \tan\left(\frac{\phi}{2}\right)\sin(N+n)\phi \cdot \sin(N-n)\phi.$$ 

2) A few impurities problem

Let us consider a case where there are several impurities separated each other by a finite number of host atoms. For example, consider that three isotopic impurities are inserted into the chain. Three types of localized modes may then appear. The first type is caused by the divergence of each of $S$-matrices associated with three isotopes and has a shape produced by a superposition of three waves which damp exponentially with increasing distance from the impurities. The second is caused by the divergence of both the propagator between a pair of neighboring impurities and the $S$-matrix of the remaining isotope. The third corresponds to the divergence of the propagator between three isotopes. Actually, however, only the last type can occur. The following consideration excludes the former two possibilities. In the second type, the localized wave trapped between two neighboring isotopes damps exponentially towards the remaining isotope. Because of the finite separation between them, a tail of the wave is not zero at the isotope. Then the wave must be smoothly joined at the isotope to a wave which diverges exponentially towards the other side. It is not physical. The same reasoning is valid also for the first type.

As examples of the application of $S$-matrix method to the case of a few impurities, only following two cases are considered.

a) Localized mode trapped between two isotopic impurities

Two isotopic impurities are inserted in the infinitely extended chain, with the interval of $(n-1)$ host atoms. The associated $S$-matrix product is

$$\cdots \begin{pmatrix} e^{i\phi} & a \\ 1-a & 1-a \end{pmatrix} \begin{pmatrix} i^n a \\ e^{i\phi} \end{pmatrix} \begin{pmatrix} 1-a & 0 \\ e^{-i\phi} & 1-a \end{pmatrix} \begin{pmatrix} i^n a \\ e^{i\phi} \end{pmatrix} \cdots.$$ 

The inverse of the propagator is easily found to be

$$1 - \left( \frac{ae^{2in\phi}}{1-a} \right)^2.$$ 

After some calculations, $z$ comes out to be determined by the equation

$$e^z = \frac{2-Q}{Q} = \pm (-1)^n \frac{1-Q}{Q} (1+e^z)e^{-nz}.$$
For $n=1$, the above equation becomes

$$a = \frac{e^x}{e^x \pm 1}, \quad \text{where } a = (1-Q) \coth \left( \frac{z}{2} \right).$$

Changing a variable form $z$ to $x=e^z$, we get two pairs of the simultaneous equations

$$\begin{cases}
y = 1 - Q + \frac{2(1-Q)}{x-1} \\
y = 1 - \frac{1}{x+1}
\end{cases}, \quad \begin{cases}
y = 1 - Q + \frac{2(1-Q)}{x-1} \\
y = 1 + \frac{1}{x-1}
\end{cases}$$

The solutions of the above equations can be obtained graphically. The solution of the equation $a = e^x(e^x + 1)^{-1}$ always exists when $0 < Q < 1$, while the solution of $a = e^x(e^x - 1)^{-1}$ exists only when $0 < Q < 1/2$.

As is shown in Appendix A, the former corresponds to the antisymmetric mode, and the latter to the symmetric mode.

b) Localized mode trapped between two isotopic impurities at the free boundary

In the case sketched in Fig. 6, the associated S-matrix is obtained from the product

$$\cdots \left( \frac{e^{i\varphi}}{1-a} \frac{a}{1-a} \right)^3 \left( \begin{array}{cc} 0 & 1 \\ e^{i\varphi} & 0 \end{array} \right).$$

On setting $\varphi = \pi + iz$ and changing a variable form $z$ to $x=e^z$, we obtain the following equation which gives the values of $z$ corresponding to localized modes:

$$\frac{ax}{1-a} + \left( \frac{x}{1-a} \right)^2 \frac{a}{1-a} x \left(1 - \left( \frac{ax}{1-a} \right)^{-1} \right) = -1,$$

where

$$a = -(1-Q) \frac{x+1}{x-1}.$$

After some calculations this equation becomes

$$(1+x)^s Q^s - \{2(1+x)^s - (x^2 + x + 2)(x+1)\} Q + (1+x)^s$$

$$- (x^2 + x + 1)(x+1) + 1 = 0.$$

Solving the above equation, we get finally the relation
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\[ Q = \frac{x + 3 \pm \sqrt{x^2 + 2x + 5}}{8 \cosh^2 \left( \frac{z}{2} \right)}. \]

3) Generalized island

Let us finally consider the case in which \(2n\) isotopic impurities are inserted in the infinitely extended chain with an equal interval of \((m-1)\) host atoms. The argument can readily be generalized to the case of odd number of impurities. The S-matrix of an element is found to be

\[
\begin{pmatrix}
    e^{i\theta} & 0 \\
    0 & e^{i\phi}
\end{pmatrix}^{m-1}
\begin{pmatrix}
    e^{i\theta} & a \\
    1-a & 1-a
\end{pmatrix}
\begin{pmatrix}
    e^{i\phi} & a \\
    1-a & 1-a
\end{pmatrix}^* =
\begin{pmatrix}
    e^{i\theta} & a \\
    1-a & 1-a
\end{pmatrix}
\begin{pmatrix}
    e^{i\phi} & a \\
    1-a & 1-a
\end{pmatrix}^*.
\]

Then the localized modes are found by the equations

\[ \sinh (2n\delta) - t \sinh (2n-1)\delta = 0, \]

and

\[ 2t \cosh \delta = 1 + t^2 - \rho^2. \]

From the last equation, we obtain

\[ (-1)^m \cosh \delta = \cosh (mz) - (1 - Q) \coth \left( \frac{z}{2} \right) \sinh (mz). \]

Solving this, \(\cos \delta\) can be represented in terms of \(\cos x\).

On the other hand, if we define

\[ f(\cos \delta) = \frac{\sinh (2n\delta)}{\sinh (2n-1)\delta} \]

\[ = 2 \cos \delta \Pi \left( \cos \delta - \cos r \epsilon \right) \left( \cos \delta + \cos r \epsilon' \right), \]

where

\[ \epsilon = \frac{\pi}{2n}, \quad \text{and} \quad \epsilon' = \frac{\pi}{2n-1}, \]

then the values of \(x\) corresponding to the localized modes are determined by the intersections of the curves \(f(\cos x)\) and

\[ t = \frac{(-1)^m e^{-m\epsilon}}{1 - (1 - Q) \coth \left( \frac{z}{2} \right)}. \]

If \(2n-1\) impurities are inserted, \(f(\cos \delta)\) becomes
\[ f(\cos \delta) = \frac{\sinh(2n-1)\delta}{\sinh(2n-2)\delta} = 2 \cosh \delta \prod_{r=1}^{n-1} \left( \frac{\cosh^2 \delta - \cos^2 r \epsilon'}{\cosh^2 \delta - \cos^2 r \epsilon''} \right), \]

where

\[ \epsilon'' = \frac{\pi}{2n-2}. \]

Thus the results for the case of odd number of impurities are easily deduced from those for the case of even number of impurities by replacing \((\epsilon, \epsilon')\) by \((\epsilon', \epsilon'')\).

a) The case \(m=1\)

In this case \(\cos \delta\) is expressed in terms of \(\cos \gamma\) as

\[ \cos \delta = 1 - Q - Q \cos \gamma. \]

Inserting the above relation in \(f(\cos \delta)\), we get

\[ f(\cos \gamma) = -2Q \left( \cosh \gamma - \frac{1-Q}{Q} \right) \prod_{r=1}^{n-1} \left( \frac{\cos \gamma - \alpha_r^{(\ast)}}{\cos \gamma - \beta_r^{(\ast)}} \right), \]

where

\[ \alpha_r^{(\ast)} = \frac{1-Q}{Q} + \frac{\cos r \epsilon}{Q}, \quad \alpha_r^{(-)} = \frac{1-Q}{Q} - \frac{\cos r \epsilon}{Q}, \]

\[ \beta_r^{(\ast)} = \frac{1-Q}{Q} + \frac{\cos r \epsilon'}{Q}, \quad \beta_r^{(-)} = \frac{1-Q}{Q} - \frac{\cos r \epsilon'}{Q}. \]

Comparing the magnitudes of \(\alpha\)'s and \(\beta\)'s, we get the sequence

\[ \frac{2-Q}{Q} > \alpha_1^{(\ast)} > \beta_1^{(\ast)} > \cdots > \alpha_{n-1}^{(\ast)} > \beta_{n-1}^{(\ast)} > \alpha_n^{(-)} > \beta_n^{(-)} > \cdots > \alpha_l^{(-)} > \alpha_l^{(\ast)} > -1, \]

where

\[ \alpha_* = \frac{1-Q}{Q}, \]

while \(t\) is given in terms of \(\epsilon'\) as

\[ t = \frac{1 - \epsilon'}{Q \epsilon'' - (2-Q) \epsilon'}. \]

The number of intersection is equal to the number of \(\alpha\)'s which are larger than 1.

In the case \(1/2 < Q < 1\), only the \(\alpha^{(\ast)}\)'s which satisfy

\[ \frac{1-Q}{Q} + \frac{\cos \bar{\epsilon}}{Q} > 1, \quad \text{or} \quad \cos \bar{\epsilon} > 2Q - 1, \]

are larger than 1. Here \(\bar{\epsilon} = \pi/N, N\) being the number of impurities. The
number of the localized modes is given by the number of integers which satisfies the above condition.

In the case $Q<1/2$, all the $\alpha_{\ell}^{(+)}$s become larger than 1. The number of integers which satisfies the condition

$$\frac{1-Q}{Q} - \frac{\cos r\bar{e}}{Q} > 1,$$

or

$$\cos r\bar{e} < 1 - 2Q$$

gives the number of $\alpha_{\ell}^{(+)}$s which are larger than 1 and also the number of the corresponding localized modes. Especially, for $N$ localized modes to appear, the following condition must be satisfied

$$\cos \left( \frac{\pi}{N} \right) < 1 - 2Q.$$

b) The case $m=2$

The relation between $\delta$ and $z$ becomes

$$\cosh \delta = 2Q \cosh^2 x - 2(1 - Q) \cosh z - 1.$$

Inserting this relation to $f'(\cos \delta)$, we get

$$f(x) = 4Q \prod_{r=1}^{\infty} \frac{x - \alpha_{r}^{(+)} + x - \alpha_{r}^{(-)} - x - \mu_{r}^{(+)} + x - \mu_{r}^{(-)}}{x - \beta_{r}^{(+)} + x - \beta_{r}^{(-)} - x - \nu_{r}^{(+)} + x - \nu_{r}^{(-)}} (x - \alpha_{s})(x - \mu_{s}),$$

where

$$\alpha_{r}^{(\pm)} = \frac{1 - Q + \sqrt{(1 - Q)^2 + 2Q(1 \pm \cos r\bar{e})}}{2Q},$$

$$\mu_{r}^{(\pm)} = \frac{1 - Q - \sqrt{(1 - Q)^2 + 2Q(1 \pm \cos r\bar{e})}}{2Q},$$

$$\beta_{r}^{(\pm)} = \frac{1 - Q + \sqrt{(1 - Q)^2 + 2Q(1 \pm \cos r\bar{e})}}{2Q},$$

$$\nu_{r}^{(\pm)} = \frac{1 - Q - \sqrt{(1 - Q)^2 + 2Q(1 \pm \cos r\bar{e})}}{2Q}.$$

Comparing the magnitudes of $\alpha$'s, $\beta$'s, $\mu$'s and $\nu$'s, we get the following sequences.

$$\frac{1}{Q} > \alpha_{1}^{(+)} > \beta_{1}^{(+)} > \cdots > \alpha_{s}^{(+)} > \beta_{s}^{(+)} > \alpha_{s}^{(-)} > \beta_{s}^{(-)} > \alpha_{s-1}^{(+)} > \cdots > \alpha_{1}^{(-)} > \frac{1-Q}{Q},$$

$$0 > \mu_{1}^{(+)}, \nu_{1}^{(+)}, \cdots > \mu_{s-1}^{(+)}, \nu_{s-1}^{(+)}, \mu_{s-1}^{(-)}, \nu_{s-1}^{(-)}, \cdots > \nu_{1}^{(-)} > \mu_{1}^{(-)} > 1,$$

where

$$\alpha_{s} = \frac{1 - Q + \sqrt{1 + Q^2}}{2Q}.$$
\[
\mu_\ast = \frac{-1 - Q - \sqrt{1 + Q^2}}{2Q}.
\]

According to the dispersion relation
\[
\omega^2 = \omega_0^2 \frac{1 + \cos \varphi}{2},
\]
\(z=1/Q\) corresponds to \(\omega = 2\tau / (1 + M + 1/M')\), and \(z=(1-Q)/Q\) to \(\omega = 2\tau / M'\), and 0 to \(2\tau / M\), and \(-1\) to 0.

In the case \(3/4 < Q < 1\), the number of integers which satisfy the condition
\[
\cos \varphi \tilde{e} > 4Q - 3
\]
is just the number of localized modes which come out from the top of the band of the perfect chain.

In the case \(1/2 < Q < 3/4\), all \(\alpha^+(\varphi)^3\)'s become larger than 1, and the condition
\[
\cos \varphi \tilde{e} < 3 - 4Q
\]
determines the number of localized modes the frequencies of which are smaller than the one corresponding to \(\alpha_\ast\).

Finally, in the case \(Q < 1/2\), the maximum number of localized modes come out from the top of the band of the perfect chain, to form an impurity band.

**Acknowledgements**

The authors wish to express their thanks to Professors M. Toda, J. Hori, S. Ono, N. Saito and all the other members for valuable discussion at the “Fourth Symposium on the Theory of Lattice Vibrations of Imperfect Crystals”.

**Appendix A**

*The symmetric and antisymmetric localized modes of two adjacent impurities*

Suppose that there is a localized wave trapped between two adjacent impurities specified by the same scattering matrix \((t, \tau, r, \rho)\). Waves at host atoms damp exponentially with increasing distance from impurities. The vibration of each impurity has an incoming part, but an outgoing part, or a reflected wave, exists only in the vibration of one impurity, as for example is seen in Fig. 7. Then the complex amplitudes \(z_i\)'s are connected by the following linear transformation
The symmetric mode requires the following relation

$$z_1 + z_2 = z_3$$

which leads to the condition:

$$\frac{1}{t} + \frac{r}{t} = 1.$$

Similarly the condition for the antisymmetric mode

$$z_1 + z_2 = -z_3$$

leads to

$$\frac{1}{t} + \frac{r}{t} = -1.$$

In the case of isotopic impurity, these conditions reduce to

$$1 + \frac{ae^{i\varphi}}{1-a} = \pm \frac{e^{i\varphi}}{1-a},$$

Together with the localized mode condition

$$\left(\frac{ae^{i\varphi}}{1-a}\right)^2 = 1,$$

and

$$\varphi = \pi + iz,$$

we get

$$a = \frac{e^i}{e^i + 1},$$

where

$$a = (1 - Q) \coth \frac{z}{2},$$

and the minus sign corresponds to the symmetric mode and the plus sign to the antisymmetric mode.
Appendix B

Solution of the difference equation for $\rho_*$

In the difference equation

$$\rho_{n+1} = \rho + \frac{t^2}{1-\rho^*} \rho_* ,$$

we change the variable $\rho_*$ to the variable $g_*$ given by the relation

$$1-\rho^* = \frac{g_{n+1}}{g_*} .$$

Then the difference equation becomes

$$g_{n+2} - (2t \cosh \delta) g_{n+1} + t^2 g_* = 0 ,$$

where

$$2t \cosh \delta = 1 + t^2 - \rho^* .$$

If we put

$$g_* = C \beta^*$$

and substitute in the equation, this becomes

$$\beta^2 - (2t \cosh \delta) \beta + t^2 = 0 .$$

Thus we have

$$\beta = t (\cosh \delta \pm \sinh \delta) ,$$

and

$$g_* = C_1 t^n (\cosh \delta + \sinh \delta)^n + C_2 t^n (\cosh \delta - \sinh \delta)^n .$$

From the initial conditions

$$g_0 = 1, \text{ and } g_1 = 1 ,$$

$C_1$ and $C_2$ are found to be

$$C_1 = \frac{1 - t (\cosh \delta - \sinh \delta)}{2t \sinh \delta} ,$$

$$C_2 = \frac{t (\cosh \delta + \sinh \delta) - 1}{2t \sinh \delta} .$$

Then an complete expression of $g_*$ is obtained and after some algebraic calculations $\rho_*$ is found to be
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\[ \rho_* = \frac{1}{r} \left( 1 - \frac{g_{s+1}}{g_*} \right) \]

\[ = \frac{\rho \sinh(n\delta)}{\sinh(n\delta) - t \sinh(n-1)\delta} \cdot \]

References