Operator Method for Solving the Difference Equations

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Abstract: - Very-effective method of solving of difference equations is the operator’s one, where the operators are the translational ones. It is demonstrated how this method gives the solution of the second order equation with variable function. The solution is applicable to investigation of Frenkel’s excitons behavior in thin molecular film.

Key-words: - Translational operators, General solution, Frenkel’s excitons, Thin films.

1 Introduction

Difference equations (see [1-5]) play important roll in condensed matter physics, especially in the problems connected with crystal structures. Probability amplitudes in one-particle wave function as well as Green’s functions are the solutions of systems of difference equations. A general type of difference equations defining mentioned quantities is the following:

\[ Y_{n+1} + Y_{n-1} + \rho_n Y_n = 0, \]

(1)

where integer \( n \) denotes place of atom or molecule, while \( \rho \) is parameter consisting physical characteristic of system.

If crystal structure is translational invariant (see [6]), parameter \( \rho \) does not depend on integer \( n \). In the cases of broken symmetry (impurities, presence of boundaries etc.), this parameter \( \rho \) is dependent on molecule position \( n \). In the mentioned cases difference equation (1) goes over to equation with variable coefficient \( \rho \), i.e.

\[ Y_{n+1} + Y_{n-1} + \rho_n Y_n = 0. \]

(2)

It should be pointed out that the equations (1) and (2) are written in the nearest neighbor’s approximation. If we take into account the next nearest neighbor’s approximation or still more exact case (we can take all neighbors into account) the quoted equations (1) and (2) are changing and parameter \( \rho \) is also changed. The fundamental characteristics of parameter \( \rho \), independently on the approximation used, is the fact that it contains energy of elementary excitations. The probability amplitudes are also dependent on \( \rho \). It should be noticed that equation (2) could have two types of solutions: periodical and aperiodical. If the solution is periodical, excitations are uniformly distributed in all crystal. For aperiodical solution excitations are localized close the deformation. The model is valid for cubic structures in the nearest neighbor’s approximation. In the case of excitons in molecular crystal with dipole-dipole interactions those decrease with the distance \( |\bar{n} - \bar{m}| \) between molecules by the rule \( |\bar{n} - \bar{m}|^{-3} \). The nearest neighbor’s approximation in this case is under border of allowed but it is often used because the interaction between molecules are for two order of magnitude
less than the excitation energy of an isolated molecule.

In thin film, the excitations corresponding to \( \rho \) which is expressed through aperiodical function are localized near surface layers of the film and they are called “surface states” (see [7,8]).

In the second section of this work the general procedure of solving the equation (2) will be exposed. A particular example will be solved, too.

2 Solution of the general difference equation describing crystal structure with broken symmetry

In the introductory part a difference equation with parameter depending on molecule position \( n \) was quoted. It means that we shall solve the equation of the form (2). The equation (2) will be solved using operator's method. The application of this method requires introduction of translation operators \( \hat{T}_i \) obeying the following rules:

\[
\hat{T}_i f_n = f_{n+1}; \quad \hat{T}_i \hat{T}^{-1}_i = \hat{T}^{-1}_i \hat{T}_i; \quad \hat{T}_i \hat{T}^{-1}_j = \hat{T}^{-1}_j \hat{T}_i; \quad \hat{T}_0 = 1
\]

(3)

Taking into account (3) the equation (2) can be written in the form:

\[
\left( \hat{T}_i + \hat{T}^{-1}_i + \rho_n \right) Y_n = 0
\]

(4)

Operator’s solving requires that at least one of the left-hand side operators in (4) gives zero acting to constant. It is easily seen that none of the operators, i.e. \( \hat{T}_i + \hat{T}^{-1}_i \) and \( \hat{\rho}_n \) do not satisfy this requirement. Therefore we shall transform (4) in the following way:

\[
\left( \hat{T}_i + \hat{T}^{-1}_i \right)^2 + \hat{\rho}_n Y_n = 0
\]

(5)

It is seen now that translational operator \( \hat{T}_i + \hat{T}^{-1}_i \) acting to constant gives zero, i.e.

\[
\left( \hat{T}_i + \hat{T}^{-1}_i \right)^2 C = \hat{T}_i C + \hat{T}^{-1}_i C - 2C = 0
\]

(6)

In this way the operator form in (5) is prepared for application of operator method.

In order to make calculations more clear and compact, we shall introduce the following notations:

\[
\hat{a} = \hat{T}_i + \hat{T}^{-1}_i - 2
\]

(7)

and

\[
\hat{b}_n = \hat{\rho}_n + 2.
\]

(8)

The equation (2.4) now has the form:

\[
\left( \hat{a} + \hat{b}_n \right) Y_n = 0
\]

(9)

The operator’s method gives the solution of homogenous difference equation expressed over two linearly independent solutions of the corresponding non-homogenous equation:

\[
\left( \hat{a} + \hat{b}_n \right) Y_n = \Phi_n
\]

(10)

Really, if (10) has two linearly independent solution, \( y_n^{(1)} \) and \( y_n^{(2)} \), then the following is valid:

\[
\left( \hat{a} + \hat{b}_n \right) y_n^{(1)} = \Phi_n
\]

\[
\left( \hat{a} + \hat{b}_n \right) y_n^{(2)} = \Phi_n
\]

Subtracting these equations we obtain:

\[
\left( \hat{a} + \hat{b}_n \right) (y_n^{(1)} - y_n^{(2)}) = 0
\]

(11)

Comparing (11) with (9) we conclude that:

\[
y_n = y_n^{(1)} - y_n^{(2)}
\]

(12)

The further question is how to find the functions \( y_n^{(1)} \) and \( y_n^{(2)} \)? The formal solution of (2.9) is:

\[
y_n = (\hat{a} + \hat{b}_n)^{-1} \Phi_n
\]

(13)

Now, it can be shown that there do exist two independent forms of the operator \( (\hat{a} + \hat{b}_n)^{-1} \). First it is clear that the operator \( \hat{a} + \hat{b}_n \) can be written in two different ways:

\[
\hat{a} + \hat{b}_n = \begin{pmatrix} \hat{b}_n (1 + \hat{b}_n^{-1} \hat{a}) \\ \hat{a} (1 + \hat{a}^{-1} \hat{b}_n) \end{pmatrix}
\]

(14)

wherefrom it follows that:

\[
(\hat{a} + \hat{b}_n)^{-1} = \begin{pmatrix} [1 + \hat{b}_n^{-1} \hat{a}]^{-1} \hat{b}_n^{-1} - \sum_{k=0}^{\infty} (-1)^k \hat{b}_n^{-k} \\ [1 + \hat{a}^{-1} \hat{b}_n]^{-1} \hat{a}^{-1} - \sum_{k=0}^{\infty} (-1)^k \hat{a}^{-k} \hat{b}_n \end{pmatrix}
\]

(15)

Since the translational operator \( \hat{a} \) and multiplicative operator \( \hat{b}_n \) do not commutate, \( n \)th power of the product of such operators must be taken in accordance with the rule:

\[
[\hat{F}, \hat{G}] \neq 0 : \prod_{n = \text{times}} \hat{F} \hat{G} \hat{F} \hat{G} \ldots \hat{F} \hat{G}
\]

(16)

Taking into account (13) and (15) we have:

\[
y_n^{(1)} = (1 - \hat{b}_n^{-1} \hat{a} + \hat{b}_n^{-2} \hat{a} \hat{b}_n^{-1} \hat{a} - \ldots) \hat{b}_n^{-1} \Phi_n
\]

(17)

and

\[
y_n^{(2)} = (1 - \hat{a}^{-1} \hat{b}_n + \hat{a}^{-2} \hat{b}_n \hat{a}^{-1} \hat{b}_n - \ldots) \hat{a}^{-1} \Phi_n
\]

(18)

If we take that \( \Phi_n = \hat{b}_n \), then it follows from (17):

\[
y_n^{(1)} = 1
\]

(19)

In the same time (2.17) gives:
\( y^{(2)}_n = \hat{a}^{-1} \hat{b}_n - \hat{a}^{-1} \hat{b}_n \hat{a}^{-1} \hat{b}_n + \hat{a}^{-1} \hat{b}_n \hat{a}^{-1} \hat{b}_n \hat{a}^{-1} \hat{b}_n - \ldots \) (20)

Taking into account formulae (11), (19) and (20), we conclude that the solution of homogenous equation (12) is given as follows:

\( Y = 1 - \hat{a}^{-1} \hat{b}_n + \hat{a}^{-1} \hat{b}_n \hat{a}^{-1} \hat{b}_n - \hat{a}^{-1} \hat{b}_n \hat{a}^{-1} \hat{b}_n \hat{a}^{-1} \hat{b}_n - \ldots \) (21)

We can find now the explicit form of the operator \( \hat{a}^{-1} \).

Since:

\[
\begin{align*}
\hat{a} &= -2 \left[ 1 - \frac{1}{2} (\hat{T}_1 + \hat{T}_{-1}) \right] \\
&\quad \left[ (\hat{T}_1 + \hat{T}_{-1}) - 2(\hat{T}_1 + \hat{T}_{-1})^{-1} \right]
\end{align*}
\]

we have two forms of inverse operator:

\[
(\hat{a}^{-1})_1 = \hat{z}_1 = -\sum_{k=0}^{\infty} \frac{1}{2^{k+1}} (\hat{T}_1 + \hat{T}_{-1})^k
\]

and

\[
(\hat{a}^{-1})_2 = \hat{z}_2 = \sum_{k=0}^{\infty} 2^k (\hat{T}_1 + \hat{T}_{-1})^{-(k+1)}
\]

It is seen that in (24) figure powers of the operator \((\hat{T}_1 + \hat{T}_{-1})^{-1}\). This operator can be written in two ways. Since:

\[
(\hat{T}_1 + \hat{T}_{-1}) = \left[ \hat{T}_1 (1 + \hat{T}_{-2}) \right] (1 + \hat{T}_2)
\]

we obtain

\[
\left[ (\hat{T}_1 + \hat{T}_{-1})^{-1} \right]_1 = \theta_1 = \sum_{k=0}^{\infty} (-1)^k \hat{T}_{-2k-1}
\]

and

\[
\left[ (\hat{T}_1 + \hat{T}_{-1})^{-1} \right]_2 = \theta_2 = \sum_{k=0}^{\infty} (-1)^k \hat{T}_{2k+1}
\]

Now, all necessary elements for application for operator method are given. The method described will be tested on one particular example.

We shall consider difference equation

\[
Y_{n+1} + Y_{n-1} + (Ae^{an} - 2)Y_n = 0
\]

This equation can be written as

\[
(\hat{a} + \hat{b}_n)Y_n = 0
\]

with

\[
\hat{b}_n = Ae^{an}
\]

On the basis of the formula (2.20) the solution of (28) is given by:

\[
Y = 1 - \hat{a}^{-1} Ae^{an} + \hat{a}^{-1} Ae^{an} \hat{a}^{-1} Ae^{an} - \ldots
\]

Now, we shall look for the function \( \hat{a}^{-1} Ae^{an} \) using for the operator \( \hat{a}^{-1} \) the formula (24). It is clear that, since

\[
(\hat{T}_1 + \hat{T}_{-1}) Ae^{an} = 2Ae^{an} \cosh \alpha
\]

it has to be

\[
(\hat{T}_1 + \hat{T}_{-1})^{-1} Ae^{an} = \frac{1}{2 \cosh \alpha} Ae^{an}
\]

(33) we can write:

\[
\hat{a}^{-1} Ae^{an} = \left( \hat{T}_1 + \hat{T}_{-1} \right)^{-1} Ae^{an} + 2(\hat{T}_1 + \hat{T}_{-1})^{-2} Ae^{an} + \ldots
\]

\[
= \frac{Ae^{an}}{2 \cosh \alpha} + \frac{Ae^{an}}{2 \cosh^2 \alpha} + \frac{Ae^{an}}{2 \cosh^3 \alpha} + \ldots
\]

\[
= \frac{Ae^{an}}{2 \cosh \alpha} \left( 1 + \frac{1}{\cosh \alpha} + \frac{1}{\cosh^2 \alpha} + \ldots \right)
\]

\[
Ae^{an} \cosh \alpha \cosh \alpha - 1
\]

Further we have:

\[
\hat{a}^{-1} Ae^{an} \hat{a}^{-1} Ae^{an} = \hat{a}^{-1} Ae^{an} \frac{Ae^{an}}{2(\cosh \alpha - 1)}
\]

\[
= A^2 e^{2an} \frac{2}{(\cosh \alpha - 1)}
\]

wherefrom it can be easily concluded that the solution (28) is given as follows:

\[
Y_n = 1 + \sum_{k=1}^{\infty} (-1)^k \left( \frac{Ae^{an}}{2} \right)^k \frac{1}{\prod_{s=1}^{k} (\cosh s \alpha - 1)}
\]

(35)

Ending the analyses of the illustrative example (28) we shall prove that (35) identically satisfies (28). It is seen that the sum of the first, second and fourth term of (28) is:

\[
\sum_{k=1}^{\infty} (2 \cosh s \alpha - 2) (-1)^k \left( \frac{Ae^{an}}{2} \right)^k \frac{1}{\prod_{s=1}^{k} (\cosh s \alpha - 1)}
\]

The third term in (28) can be written as

\[
\sum_{k=1}^{\infty} (-1)^{k+1} \left( \frac{Ae^{an}}{2} \right)^{k+1} \frac{2 \cosh (k+1) \alpha - 1}{\prod_{s=1}^{k+1} (\cosh s \alpha - 1)}
\]

After the substitution \( k + 1 = k' \rightarrow k \) this term reduces to:

\[
\sum_{k=1}^{\infty} (-1)^k \left( \frac{Ae^{an}}{2} \right)^{k+1} \frac{2 \cosh k \alpha - 1}{\prod_{s=1}^{k} (\cosh s \alpha - 1)}
\]

and consequently the solution (35) identically satisfies (28).
3 Conclusion

The main part of this work is rather of methodological character: the method of operator solving of basic solid-state difference equation with variable coefficient is demonstrated there. Unfortunately this method gives the compact solution if the variable coefficient is of exponential type. In other cases the method is also applicable but solutions are clumsy. Therefore, in such cases it is better to apply numerical calculation using the formula (21) quoted in the Section 2. The example, which is solved in Section 2, can be applied to the problem of molecular displacements in one dimension chain with intermolecular distances which are minimal at the beginning of the chain and which are exponentially increasing in the direction of the second end of the chain.

References: