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Floquet Bloch Theory Used to Analyze the Stability of Periodic Systems

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Abstract – This study, the role and effects of Floquet Bloch theory on partial differential equations with periodic coefficients were investigated. Results are given about the Floquet expansions of arbitrary solutions, the solvability of non-homogeneous equations, the existence and structure of solutions, especially for boundary value problems that arise in applications of Schrödinger equations. This theory is of great importance for the quantum theory of solids, the theory of waveguides, scattering theory and other fields of mathematical and theoretical physics.

Keywords – Floquet Bloch Theory, Spectrum, Solvability, Non-Homogeneous, Schrödinger Equations

I. Introduction

Floquet-Bloch theory appears in mechanical systems. It is a theory that deals with wave propagation problems. In layered systems, the heterogeneity feature of elastic structures enables certain wave patterns to physically propagate throughout the structure [1]. These models are defined by a function of time frequency and wavenumber and are generally nonlinear. The curves given in this way are called distribution curves and affect the entire oscillatory behavior of the system. Therefore, their calculation is very important in applying the equations [2].

Vibrations are also prominent in objects with a periodic structure [3]. These problems are usually divided into time- and space-dependent parts of the solution. For example, the Helmholtz equation corresponds to an equation that describes spatial behavior [4]. Here the physical periodic structure of the object under study translates into the periodicity of its coefficients. Therefore, Floquet-Bloch theory has found different applications to study and investigate the distribution properties of different mechanical periodic systems [5], [6]. Many structures, mostly civil engineering structures [2], [3], optical [10], [11], or electromagnetic [12], can be considered as infinitely large layered systems. In periodic systems controlling electronic devices, vibroacoustic diffusion of waves has been optimized to calculate wave dispersion in damped mechanical systems [13]. Numerical approaches to this calculation are modeled in the direction of wave propagation by applying the finite element method and using a harmonic function [14]. An eigenvalue problem is modeled by introducing the displacement field into the auxiliary equations. Solving the eigenvalue problem for a given frequency serves to obtain the wave numbers of all propagation modes.

In this study, the role and effects of Floquet Bloch theory for partial differential equations with periodic coefficients are investigated. In particular, boundary value problems that arise in applications for Schrödinger equations are investigated, and results are given about the completeness of the Floquet solution set, Floquet expansions of arbitrary solutions, and the solvability of non-homogeneous equations. This theory is of great importance for the quantum theory of solids, the theory of waveguides, scattering theory and other fields of mathematical and theoretical physics.

II. Materials and Method

The Schrödinger Equation in a Periodic Potential

Four Schrödinger equations can be written for a particle of mass m in the periodic potential $V(x)$.

$$H\varphi = \{\frac{-h^2\nabla^2}{2m} + V(x)\}\varphi = E\varphi . \quad (1)$$

Here we write the potential as a Fourier series

$$V(x) = \sum_P V_P e^{iPx}, \quad (2)$$

where P are mutual lattice vectors. We can determine the source of potential energy wherever we want. To make subsequent derivations easier, let's take the potential as $V_0 = 0$.

We can write the wave function ψ as the sum of plane waves obeying the Born-von Karman conditions,

$$\varphi(x) = \sum_k C_k e^{ikx} \quad (3)$$

This ensures that ψ also obeys the Born-von Karman boundary conditions. Now, by substituting the wave equation in (3) and the potential equation in (2), we will obtain the Schrödinger equation in (1),

$$\sum_k \frac{h^2k^2}{2m} C_k e^{ikx} + \{\sum_P V_P e^{iPx}\}\{\sum_k C_k e^{ikx}\} = E\sum_k C_k e^{ikx}. \quad (4)$$

If we rewrite the potential energy

$$V(x)\varphi = \sum_{P,k} V_P C_k e^{i(k+P)x}, \quad (5)$$

where the sum on the right side is over P and k. Sum, can be rearranged as follows,

$$V(x)\varphi = \sum_{P,k} V_P C_{k-P} e^{ikx}, \quad (6)$$

Therefore the Schrödinger equation in (4) becomes

$$\sum_k e^{ikx}((\frac{h^2k^2}{2m} - E) C_k + \sum_P V_P C_{k-P}) = 0.$$

Since Born-von Karman plane waves are a set of orthogonal functions, the coefficient of each term is the sum must be zero (we can get this by multiplying by a plane wave and integrating), so,

$$\left(\frac{h^2k^2}{2m} - E\right) C_k + \sum_P V_P C_{k-P} = 0. \quad (7)$$

(7) is taken as $V_P = 0$. It would be convenient to deal only with solutions in the first Brillouin zone (anyway we can see that this gives all the necessary information about the k-space). So we write $k = (q - P')$, where q is in the first Brillouin zone and P' is the reciprocal lattice vector. Equation in (7) can then be rewritten

$$\left(\frac{h^2(q-P')^2}{2m} - E\right) C_{q-P'} + \sum_P V_P C_{q-P'-P} = 0.$$

Here, if we change the variables to be $P'' \to P + P'$,

$$\left(\frac{h^2(q-P')^2}{2m} - E\right) C_{q-P'} + \sum_P V_{P''-P'} C_{q-P''} = 0.$$

(8)

This specifies C_k, which is used to generate the wave function φ in equation (3).

Bloch's Theory

Equation in (8) includes only coefficients C_k where $k = q - P$; In other words, if we choose a particular value of q, then the only C_k found in it will have the property. Equation in (8) is in the form C_{k-P}; these coefficients specify the shape of the wave function.

Therefore, for every different value of q, there is a wave function $\varphi q(x)$ that takes the form:

$$\varphi q(x) = \sum_P C_{q-P} e^{i(q-P)x}, \quad (9)$$

We obtained the equation by substituting $k = q - P$ in equation (3). If equation (9) is rewritten

$$\varphi q(x) = e^{iqx} \sum_P C_{q-P} e^{-iPx}, \quad (10)$$

This represents a plane wave with a wave vector within the first Brillouin zone. This allows us to reach Bloch's theorem, "Eigenstates of the one-electron Hamiltonian $H = \frac{-h^2\nabla^2}{2m} + V(x)$ where $V(x + T) = V(x)$, T can be chosen as a plane for all Bravais lattice translation vectors a function with the periodicity of the wave times the Bravais lattice.

Floquet Theory

The Schrödinger equation is taken in natural units as follows and Liouville the normal form is called,

$$\frac{-h^2\nabla^2}{2m} + V(x)\}\varphi = \lambda E\varphi . \quad (11)$$

(11) ordinary differential equation it is called the time-independent Schrödinger equation. Here E eigenvalue an energy level and its eigenfunctions are the wave corresponding to a particle represents the function. We can write the Schrödinger equation given in (11) in another way as follows,

$$\varphi''(x) = (V(x) - \lambda E)\varphi(x) \quad (12)$$

The two linearly independent solutions of equation (12) are $\varphi_1(x)$ and $\varphi_2(x)$, and the general solution of the equation is their linear combination.

*Lemma 2.1.*Any two solutions of the equation (12), $\varphi_1(x)$ and $\varphi_2(x)$ a necessary and sufficient condition for linear independence is that their Wronskian is zero is that it is different.

Proof. Let's assume that $W\,[\varphi_1(x),\ \varphi_2(x)\,] \neq 0$. Let us show that it is linearly independent.
Let $\varphi_1(x)$ and $\varphi_2(x)$ be linearly dependent. That is, let c and d be constants and

$\varphi_1(x)$= c $\varphi_2(x)$ or $\varphi_2(x)$ = d $\varphi_1(x)$

$$W\,[\varphi_1(x), \varphi_2(x)] = W[c\,\varphi_2(x), \varphi_2(x)]$$
$$= c\,W\,[\varphi_2(x), \varphi_2(x)] = 0$$

is obtained. This is the contradiction. Similarly, if we take $\varphi_2(x)$ = d $\varphi_1(x)$ again the contradiction is aged. Any two linearly independent solutions of equation (11), let us show that their Wronskian is not zero.

Let $W\,[\varphi_1(x), \varphi_2(x)] = 0$. Considering the point $x_0 \in (-\infty,\ \infty)$, a_1 and a_2, let's write the following system of equations according to the numbers below.

$$\begin{aligned} a_1\varphi_1(x_0) + a_2\varphi_2(x_0) &= 0 \\ a_1\varphi'_1(x_0) + a_2\varphi'_2(x_0) &= 0, \end{aligned} \qquad (13)$$

On assumption,

$$\begin{vmatrix} \varphi_1(x_0) & \varphi_2(x_0) \\ \varphi'_1(x_0) & \varphi'_2(x_0) \end{vmatrix} = W\,[\varphi_1(x_0), \varphi_2(x_0)] = 0.$$

Since the determinant is zero, the system has at least one non-zero a_1 and a_2 there is a solution. Like this $\omega(x) = a_1\varphi_1(x) + a_2\varphi_2(x)$ becomes the solution of equation (12).

$$\omega(x_0) = 0, \omega'(x_0) = 0, \qquad (14)$$

Since it is valid for existence and uniqueness theorem according to

$$a_1\varphi_1(x) + a_2\varphi_2(x) = 0.$$

Thus, since it is shown that $\varphi_1(x)$ and $\varphi_2(x)$ are linearly dependent the contradiction is obtained. Therefore, Wronskian cannot be zero.

Let's take the basic solution system of the equation (12). As such solutions,

$$\theta(x,\lambda): \theta(0) = 1\,, \theta'(0) = 0$$
$$\varphi(x,\lambda): \varphi(0) = 0\,, \varphi'(0) = 1$$

$\Delta(\lambda) = \theta(x) + \varphi'(x)$. Let's define it as

$$\chi_1(x) = e^{-\mu(x)}\varphi_1(x),\ \chi_2(x) = e^{\mu(x)}\varphi_2(x).$$

Definition 2.2 (Floquet Formula): General solution of equation (11), c_1 and c_2 is any two constant numbers and

$$\varphi_1(x) = e^{\mu(x)}\chi_1(x), \varphi_2(x) = e^{-\mu(x)}\chi_2(x)$$

to be,

$$\varphi(x) = c_1e^{\mu(x)}\chi_1(x) + c_2e^{-\mu(x)}\chi_2(x), \qquad (15)$$

happens, this formula is called Floquet Formula.

Theorem 2.3.(Floquet Theorem):
Let $\lambda \in (-\infty, \infty)$.
i)If $|\ \Delta(\lambda)| > 2$, (12) the differential equation is unstable.
ii) If $|\ \Delta(\lambda)| < 2$, (11) the differential equation is stable.
iii) If $|\ \Delta(\lambda)| = 2$, (11) differential equation, if $\theta'(x,\lambda) = \varphi(x,\lambda) = 0$, at least one of the stable $\theta'(x,\lambda)$ and $\varphi(x,\lambda)$ if it is different from zero, it is conditionally stable.
b) If Im$\lambda \neq 0$, the differential equation (12) is unstable for this value λ.

Proof. i)If $\Delta(\lambda) > 2$,
$e^{\mu(x)}$ and $e^{-\mu(x)}$ since there are unbounded functions, for every $x \in (-\infty, \infty)$,

$$\varphi(x) = c_1e^{\mu(x)}\chi_1(x) + c_2e^{-\mu(x)}\chi_2(x),$$

are unlimited functions. Then λ is the instability point of equation (12).

If $\Delta(\lambda) < 2$, $e^{\left(\mu+i\frac{\pi}{x}\right)(x)}$ and $e^{-\left(\mu+i\frac{\pi}{x}\right)(x)}$ since there are unbounded functions, for every x,

$$\varphi(x) = c_1e^{\left(\mu+i\frac{\pi}{x}\right)(x)}\chi_1(x) + c_2e^{-\left(\mu+i\frac{\pi}{x}\right)(x)}\chi_2(x),$$

are unlimited functions. Then λ is the instability point of equation (12).

ii) If | $\Delta(\lambda$ | < 2, β_1 and β_2 are complex numbers and $\beta_1 = e^{i\alpha x}$ and $\beta_2 = e^{-i\alpha x}$; $e^{i\alpha x}$ and $e^{-i\alpha x}$ since are bounded functions;

$$\varphi_1(x) = c_1 e^{i\alpha x}\ \chi_1(x), \varphi_2(x) = c_1 e^{i\alpha x}\ \chi_2(x),$$

its functions are limited. Here λ is the stability point of equation (12).

iii) Let $\varphi^*(x)$ be a linearly independent solution of the equation (12) with $\varphi_1(x)$. Since the function $\varphi^*(x+T)$ is also the solution of (12), d_1 and d_2 are constants.

$$\varphi*(x+T) = d_1\ \varphi_1(x) + d_2\ \varphi*(x)$$

$$W\ [\varphi_1(x+T), \varphi^*(x+T)] = W\ [\varphi_1(x+T), d_1\varphi_1(x) + d_2\varphi^*(x)]$$
$$= d_1 W\ [\varphi_1(x+T), \varphi_1(x)] + d_2 W\ [y\varphi_1(x+T), \varphi^*(x)]$$
$$= d_1\beta\ W\ [\varphi_1(x), \varphi_1(x)] + d_2\ \beta\ W\ [\varphi_1(x), \varphi^* x)\ ]$$

$$W\ [\varphi_1(x+T), \varphi^* x + T)] = d_2\ \beta\ W\ [\varphi_1(x), \varphi^* x)\ ]$$

obtained. Since Wronskian is point independent $d_2\ \beta = 1$. Like this $\beta = d_2$ since

$$\varphi^*(x+T) = d_1\varphi_1(x) + \beta\varphi^*(x).$$

If $d_1 = 0$, $\varphi^*(x+T) = \beta\varphi^*(x)$ since $|\varphi^*(x+T)| = |\varphi^*(x)|$ obtained. $|\varphi^*(x)|$ onward it is a periodic function, it is limited.

Let $d1 \neq 0$. $\beta = e^{\mu x}$ where

$$\chi_1(x) = e^{-\mu(x)}\varphi_1(x)\ ,$$
$$\chi_2(x) = e^{-\mu(x)}\varphi^*(x) - \tfrac{d_1}{\beta} x\chi_1(x)$$

let it be defined as. The function $\chi_1(x)$ is periodic and the periodicity of $\chi_2(x)$can be shown as follows,

$$\chi_2(x+T) = e^{-\mu(x+T)}\ \varphi^*(x+T) - \frac{d_1}{\beta}(x+T)\chi_1(x+T)$$

$$= e^{-\mu x}e^{-\mu T}\ [d_1\ \varphi_1(x) + \beta\ \varphi * (x)] - \tfrac{d_1}{\beta} x\ \chi_1(x) - \tfrac{d_1}{\beta}\ \chi_1(x)$$

$$= e^{-\mu x}\ e^{-\mu T} d_1\ \varphi_1(x) + e^{-\mu x}\ e^{-\mu T}\ \beta\ \varphi^*(x)) - \frac{d_1}{\beta} x\ \chi_1(x) - \frac{d_1}{\beta}\ \chi_1(x)$$

$$= e^{-\mu T} d_1\ \varphi_1(x) + e^{-\mu x}\varphi^*(x) - \tfrac{d_1}{\beta} x\ \chi_1(x) - \tfrac{d_1}{\beta}\ \chi_1(x)$$

$$= \tfrac{1}{\beta} d_1\ \varphi_1(x) + e^{-\mu x}\ \varphi^*(x) - \tfrac{d_1}{\beta} x\ \chi_1(x) - \tfrac{d_1}{\beta}\ \chi_1(x) = \chi_2(x)$$

Two linearly independent solutions of equation (12) are as follows,

$$\varphi_1(x) = e^{\mu x}\chi_1(x),$$
$$\varphi^*(x) = e^{\mu x}\left\{\frac{d_1}{\beta} x\ \chi_1(x) - \frac{d_1}{\beta}\ \chi_1(x)\right\}$$

The first of these solutions, namely $\varphi_1(x)$ is limited, second solution $\varphi^*(x)$ is unlimited.

III. RESULTS

Floquet Bloch theory is a manifestation of the Schrödinger equation in the periodic potential. It is used to describe the wave function of an electron in a crystal lattice where the potential experienced by the electron is periodic in space. Here, the role and effects of Floquet Bloch theory on partial differential equations with periodic coefficients are investigated.

IV. DISCUSSION

This theory is specifically used to support the behavior of a particle moving under a uniform force. Its importance emerges in the following areas, in materials science, it is used to analyze the electronic properties of crystals. How electrons behave within the crystal structure can help determine the properties of materials and their properties, such as conductivity.

V. CONCLUSION

Boundary value problems that arise in applications of Schrödinger equations have solutions with important results. With Floquet Bloch theory, useful results are found about the completeness of solutions, Floquet expansions of arbitrary solutions and therefore the solvability of equations. This theory occupies an important place in the quantum theory of solids, the theory of waveguides, scattering theory and other fields of mathematical and theoretical physics.

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