NL2734 **Periodic Spectral Theory**

The direct problem of periodic spectral theory is that of constructing the spectral data of certain linear operators with periodic coefficients, *i.e.*, the determination of the spectrum of this operator and of the associated eigenfunctions. The inverse problem of periodic spectral theory is the problem of the reconstruction of such an operator (and thus its coefficients) from given spectral data. Although these questions can be asked for linear partial differential operators, this article focuses on linear ordinary differential operators.

The history of periodic spectral theory starts with the investigations of Sturm and Liouville on the eigenvalues of certain differential equations of second order with given boundary conditions, now referred to as Sturm-Liouville theory. Sturm and Liouville examined independently different aspects of this problem, such as the asymptotics of eigenvalues, different comparison theorems on the solutions of similar equations with different coefficients, and theorems on the zeros of eigenfunctions. For the class of equations Sturm and Liouville considered, these results imply the existence of an infinite sequence of real, increasing eigenvalues, and orthogonality of eigenfunctions corresponding to different eigenvalues. Although their investigations did not as such deal with periodic spectral theory, many of their results carry over to this case.

Consider an ordinary differential operator of order n

$$L = q_n(x)\frac{\partial^n}{\partial x^n} + q_{n-2}(x)\frac{\partial^{n-2}}{\partial x^{n-2}} + \ldots + q_1(x)\frac{\partial}{\partial x} + q_0(x), \tag{1}$$

where the coefficients $q_j(x)$, $j = 0, \ldots, n$, are periodic functions of x, sharing a common period: $q_j(x+T) = q_j(x)$, $j = 0, \ldots, n$, and $q_{n-1}(x) = 0$. They are referred to as potentials. Using this operator L define the differential equation

$$L\psi = \lambda\psi \tag{2}$$

The direct periodic spectral problem is the problem of (i) determining the set of all $\lambda \in \mathbb{C}$ for which this differential equation has at least one bounded solution, and (ii) for each such λ, the determination of all bounded solutions. There are many technical issues to be dealt with: which function space do the potentials belong to? Which function space does ψ belong to? These issues will be ignored here. Sometimes one restricts attention to periodic solutions ψ: $\psi(x+T) = \psi(x)$, or anti-periodic solutions $\psi(x+T) = -\psi(x)$. These and other choices lead to spectra that are subsets of the spectrum as obtained without making these choices.

One approach to solve the direct spectral problem is Floquet theory (Amann, 1990). Rewrite the equation (2) as a first-order linear system:

$$\boldsymbol{\psi}' = \boldsymbol{X}(x,\lambda)\boldsymbol{\psi}, \quad \boldsymbol{X}(x+T,\lambda) = \boldsymbol{X}(x,\lambda) \tag{3}$$

with $\boldsymbol{\psi}_1 = \psi(x)$. Note that from $q_{n-1}(x) = 0$ it follows that $\mathrm{tr}\boldsymbol{X}(x,\lambda) = 0$. Define the monodromy matrix of this system as $\boldsymbol{M}(x_0,\lambda) = \boldsymbol{\Psi}(x_0+T, x_0, \lambda)$, where $\boldsymbol{\Psi}(x, x_0, \lambda)$ is a fundamental matrix of (3) such that $\boldsymbol{\Psi}(x_0, x_0, \lambda)$ is the identity matrix. Thus, $\boldsymbol{M}(x_0,\lambda)$ is the operator of translating x by T: $\boldsymbol{M}(x_0,\lambda)\boldsymbol{\psi}(x) = \boldsymbol{\psi}(x+T)$. Note that $\boldsymbol{\psi}(x)$ also depends on x_0 and λ, but this dependence is suppressed here. This operation commutes with d/dx, since $\boldsymbol{X}(x,\lambda)$ is periodic in x with period T. Thus (3) has a set of solutions $\boldsymbol{\phi}(x)$ which are also eigenvectors of $\boldsymbol{M}(x_0,\lambda)$. These solutions are known as Bloch functions or Floquet functions. If the eigenvalue of $\boldsymbol{M}(x_0, \lambda)$ for any Bloch function has magnitude greater than one, than this Bloch function is unbounded as $x \to +\infty$ or $x \to -\infty$. Thus, the spectrum of (3) is the set of all λ such that at least one eigenvalue of $\boldsymbol{M}(x_0, \lambda)$ has magnitude one. The periodicity of $\boldsymbol{X}(x, \lambda) = \boldsymbol{X}(x+T, \lambda)$ and the requirement $\mathrm{tr}\boldsymbol{X}(x, \lambda) = 0$ guarantee that the spectrum is independent of the choice of x_0.

An important class of periodic spectral problems is that of self-adjoint operators. These are operators whose spectrum is contained on the real line. For self-adjoint operators, the spectrum of the periodic spectral problem consists of the union of a (possibly infinite) sequence of intervals.

For the sake of explicitness, the remainder of this article will discuss the equation (Magnus & Winkler, 1979)

$$-\psi'' + q(x)\psi = \lambda\psi, \quad q(x+T) = q(x). \tag{4}$$

Note that many of the results stated below are true for general classes of periodic spectral problems. Depending on the literature source, (4) goes by the names of Hill's equation, or (after rescaling) the time-independent Schrödinger equation. This equation is self adjoint. Its spectrum is bounded from below. It is a collection of intervals such that the length of the separating gaps between intervals $\to 0$ as $\lambda \to \infty$. Using Floquet theory, the condition for λ to be in the spectrum is found to be $|\mathrm{tr}\boldsymbol{M}(x_0, \lambda)| \leq 2$. The endpoints of the intervals are given by $|\mathrm{tr}\boldsymbol{M}(x_0, \lambda)| = 2$. Since (4) is a second-order equation, there are two linearly independent Bloch functions.

The time-independent Schrödinger equation (4) of course plays a fundamental role in quantum mechanics. In this case $q(x)$ is the potential of the system, and λ plays the role of energy. The context of solid state physics is especially relevant here, as there the potential $q(x)$ is periodic. The intervals constituting the spectrum are known as allowed (energy) bands and the gaps between them as forbidden (energy) bands.

The inverse periodic spectral problem for (4) is that of the reconstruction of $q(x)$, given a collection of spectral data. Various choices are possible for the collection of spectral data. In general, the inverse problem does not have have a unique solution, using the knowledge of one spectrum. This can be resolved by also providing the eigenfunction. However, now the collection of spectral data is unnecessarily large. It is sufficient to provide two spectra (corresponding to different boundary conditions). Together with the known analyticity properties of the eigenfunction $\psi(x)$, this determines the potential $q(x)$. This is similar to the inverse scattering method where the knowledge of the scattering data and the analyticity properties of the eigenfunction determine the potential (decaying as $|x| \to \infty$) uniquely. A major difference is that in the inverse scattering method the starting point is the asymptotic behavior as $x \to \pm\infty$. This behavior is simple, providing the efficiency of the inverse scattering method. In the periodic problem, the role of $x \to \pm\infty$ is taken over by $x = x_0$, but there is no simple asymptotic behavior, resulting in a theory which is more technical and less explicit (Dubrovin, *et al.*, 1976; Novikov, *et al.*, 1984).

This lack of explicitness for solving the inverse periodic spectral problem is to some extent resolved by the consideration of so-called finite-gap potentials. These are potentials for which the number of intervals constituting the spectrum, and thus the number of gaps separating these intervals, is finite. The simplest nontrivial such example is that of the Lamé equation

$$-\psi'' + n(n+1)\wp(x - x_c)\psi = \lambda\psi. \tag{5}$$

Here $\wp(x - x_c)$ is the Weierstrass elliptic function, x_c is a fixed complex number, and n is a positive integer. In this case, the number of gaps separating the intervals in the spectrum is n.

This classical example is a special case of a more recent theory of finite-gap potentials, whose development started with the works of Novikov (1974) and Lax (1975). They show that the stationary solutions of the n-th member of the KdV hierarchy are n-gap potentials of (4). Here the KdV hierarchy is the collection of equations of the form $u_t = \partial_x(\delta H_n/\delta u)$, where H_n is any conserved quantity of the KdV equation, $\delta H_n/\delta u$ denotes the variational derivative of H_n with respect to u (see the entry on Poisson brackets), and indices denote differentiation. It was shown soon thereafter that all finite-gap potentials of (4) were of this nature. For example, the Lamé potential with $n = 1$ is a stationary solution of the KdV equation. This gives a nonspectral characterization of the finite-gap potentials.

To solve the direct spectral problem with an n-gap potential $q_n(x)$, one first considers the direct periodic spectral problem, as stated above. It is solved using Floquet theory. The outcome is the main spectrum, consisting of n finite intervals and one infinite interval. The endpoints of these intervals are labeled λ_1, λ_2, *etc*, in increasing order, as shown in Fig. 1. At the endpoints, only one of the eigenfunctions is bounded. These eigenfunctions are periodic with period T or $2T$. There are an infinite number of isolated eigenvalues inside the interval of infinite length for which there are two bounded, periodic eigenfunctions. Next one considers the Dirichlet problem

$$\begin{cases} -\psi'' + q_n(x)\psi = \lambda\psi \\ \psi(x_0) = 0, \quad \psi(x_0+T) = 0. \end{cases} \tag{6}$$

The spectrum of this problem is referred to as the auxiliary spectrum. It is discrete, and its points $\mu_k(x_0)$, $k = 1, 2, \ldots$ depend on x_0. All but n of its points lie inside the infinite interval of the main spectrum. Each remaining point lies in a different gap of the main spectrum. This is illustrated in Fig. 1. The information contained in the main

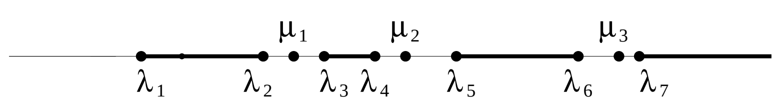

Figure 1. The main spectrum for a 3-gap potential (thick solid line) and the auxiliary spectrum μ_1, μ_2 and μ_3.

and auxiliary spectra determines the eigenfunction $\psi(x)$: it is a meromorphic function in the finite λ plane with zeros at $\lambda = \mu_k(x_0)$, and poles at $\lambda = \mu_k(x) = \mu_k(x_0)|_{x_0=x}$ (Dubrovin, *et al.*, 1976; Novikov, *et al.*, 1984).

Using the main and auxiliary spectra, the inverse periodic spectral problem is solved by (Novikov, *et al.*, 1984)

$$q_n(x) = \sum_{j=1}^{2n+1} \lambda_j - 2\sum_{j=1}^{n} \mu_j(x). \tag{7}$$

This is the first of the so-called trace formulae. Other trace formulae give relationships between the potential $q_n(x)$ and its derivatives and the main and auxiliary spectra.

The proposed solution of the inverse periodic spectral problem for finite-gap potentials is not effective. It requires the solution of the direct spectral problem for all x_0 in a period of the potential in order to obtain the auxiliary spectrum as a function of x_0. It is possible to avoid this by determining $\mu_k(x_0)$, $k = 1, \ldots, n$ as a solution of a set of differential equations (Novikov, *et al.*, 1984):

$$\frac{d\mu_j}{dx_0} = \frac{\pm 2i\sqrt{\prod_{k=1}^{2n+1}(\mu_j - \lambda_k)}}{\prod_{k\neq j}^{n}(\mu_j - \mu_k)}, \qquad j = 1, \ldots, n. \tag{8}$$

The choice of sign gives the direction in which $\mu_j(x_0)$ is going in between its two endpoints.

Another approach, which in effect solves the system (8), is the use of Abelian functions and Riemann surfaces (Dubrovin, 1981; Belokolos, *et al.*, 1994). An Abelian function of n variables is a $2n$-periodic function. As such Abelian functions generalize elliptic functions to more than one variable. All Abelian functions are expressible as ratios of homogeneous polynomials of Riemann's theta function. All finite-gap potentials of (4) are Abelian functions. For example, the Lamé potentials in (5) are elliptic functions, which are special cases of Abelian functions.

In the context of this method the Bloch function $\phi(x) = \boldsymbol{\phi}_1(x)$ is often referred to as the Baker-Akhiezer function. One of the major results of the theory is the realization that the two Bloch or Baker-Akhiezer functions, regarded as a function of arbitrary complex λ are distinct branches of one single-valued Baker-Akhiezer function, defined on a two-sheeted Riemann surface covering the complex λ plane (Krichever, 1989). This Riemann surface is already apperent in (8). It is

$$\eta^2 = \prod_{k=1}^{2n+1} (\lambda - \lambda_k), \tag{9}$$

which defines η as a double-valued function of λ. This surface has genus n. It is obtained from Fig. 1 by choosing the intervals of the main spectrum as branch cuts and gluing the two resulting sheets together along these cuts. This Riemann surface defines a theta function $\theta(z_1, \ldots, z_n|\boldsymbol{B})$ through its normalized period (or Riemann) matrix $\boldsymbol{B}$. In terms of this theta function

$$q_n(x) = c - 2\frac{d^2}{dx^2} \ln \theta(k_1 x + \varphi_1, \ldots, k_n x + \varphi_n|\boldsymbol{B}). \tag{10}$$

The wavenumbers $k_1, \ldots, k_n$ are determined as integrals of certain differentials on the Riemann surface (9) with a pole singularity at $\lambda = \infty$. The phase constants $\varphi_1, \ldots, \varphi_n$ are determined by the Riemann constants on (9) and the Abel transform. The constant c is determined by a differential on (9) with a double pole singularity at $\lambda = \infty$. Thus, (10) gives an explicit form for all finite-gap potentials of (4), providing a complete solution of the inverse periodic spectral problem.

Some remarks:

- The emphasis on finite-gap potentials is justified in the sense that any T-periodic function is approximated arbitrarily well by an infinite sequence of finite-gap potentials with period T and increasing number of gaps (Dubrovin, 1981).
- The periodic spectral problem (4) is the first half of the Lax pair for the Korteweg–de Vries (KdV) equation. As such it allows the solution of the KdV equation with

periodic initial data. The full solution of this problem requires the solution of both the direct and the inverse periodic spectral problem. The schematics is identical to that of the inverse scattering method. First, the initial condition $u(x, t = 0) = U(x)$ is used as a potential in (4) to solve the direct periodic spectral problem. This results in the main and auxiliary spectra. The time evolution of these spectra is implied from the second half of the Lax pair: the main spectrum is independent of time, whereas the auxiliairy spectrum evolves according to differential equations similar to (8). The spectral data for any time is used to solve the inverse periodic spectral problem of (4). This gives the solution $u(x, t)$ of the KdV equation such that $u(x, t)|_{t=0} = U(x)$ Novikov, *et al.* (1984).

- The spectral theory for time-dependent Schrödinger equation is intimately connected to the initial-value problem for the Kadomtsev-Petviashvili equation. A solution of the inverse periodic spectral problem using Riemann's theta function and Riemann surfaces also exists here. However, here there are no restrictions on the form of Riemann surfaces that appear: all compact, connected Riemann surfaces arise. Hence the periodic spectral theory of the time-dependent Schrödinger equation has important consequences for the theory of Riemann surfaces. It has provided, for instance, a solution to the Schottky problem, which was posed in 1903 (Novikov, *et al.*, 1984; Dubrovin, 1981).

- The equation

$$\frac{d^2y}{dx^2} + (a - 2k\cos(2x))y = 0 \tag{11}$$

is Mathieu's equation. It arises from the three-dimensional Helmholtz equation by separation of variables using elliptical coordinates. It is a special case of (4), using a trigonometric potential. One is only interested in period solutions, resulting in a discrete subset of the main spectrum. The periodic solutions of this equation are referred as Mathieu functions.

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See also Inverse scattering method; Kadomtsev-Petviashvili equation; Korteweg–de Vries equation; Theta functions.

Further Reading

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