Appendix B

Spectral theory

This chapter is devoted to the explanation of mathematical background of the spectral theory. Spectral theory of linear operators is quite widely used in linear stability or linear wave analyses in plasma physics. The mathematical basis is, however, rarely quoted in literatures, which might lead to the improper understanding of the complicated phenomena of plasmas.

The examples described here might be somewhat trivial, at least in mathematics. However, detailed analyses of basic problems may sometimes help the physicists for better understandings. First, we will review the spectral theory of finite dimensional linear matrix operator, which has been completed due to the great works by Jordan. Next, we will treat infinite dimensional differential operator, which is, in any sense, far from complete theory unlike the finite dimensional one. Since whole part of this thesis is devoted to the analyses of such infinite dimensional operators, we will focus on the simple description here and explain the basis of well-known methods widely used in literatures.

B.1 Finite dimensional operators

Let us first describe the complete classification of the finite dimensional operators. The finite dimensional operators can be classified in a suitable way for the spectral theory as follows;

1. Hermitian (selfadjoint) matrix
   All eigenvectors can be taken orthogonal and all eigenvalues are real.

2. Normal matrix (commutable with its adjoint)
   All eigenvectors can be taken orthogonal, but some eigenvalues are complex.

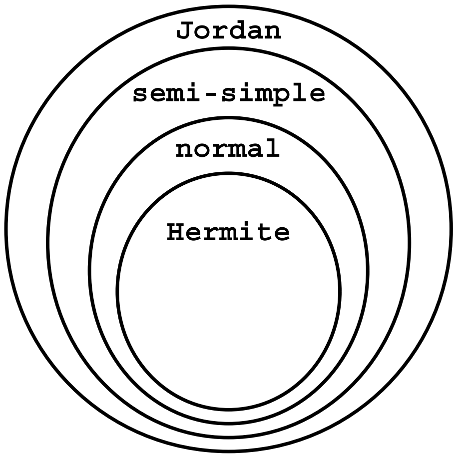

Figure B.1: Classification of finite dimensional linear matrix operators.

3. Semi-simple matrix
   Eigenvectors cannot be taken orthogonal, but linear space is spanned only by eigenvectors.

4. Jordan matrix
   Eigenvectors are not enough to span whole linear space.

The schematic view is shown in Fig. B.1. In general, any finite dimensional matrix operator belongs to one of the above sets. We can recognize how small is the region occupied by the Hermitian operators in the whole linear operators even in the finite dimensional case. In some sense, there may expand rich varieties of unknown sea out of Hermitian operators.

B.1.1 Spectral resolution of Hermitian matrices

Here we will discuss the solution of the abstract Schrödinger type evolution equation

$$\mathrm{i}\partial_t \boldsymbol{\psi} = \boldsymbol{\mathcal{A}}\boldsymbol{\psi}, \tag{B.1}$$

where the generator $\boldsymbol{\mathcal{A}}$ is assumed a Hermitian matrix defined in N ($\in \mathbb{N}$) dimensional vector space $\boldsymbol{V} = \mathbb{C}^N$. The definition of Hermitian matrix will be given later. The scalar product for two elements $\boldsymbol{\phi}, \boldsymbol{\psi} \in \boldsymbol{V}$ is defined as

$$(\boldsymbol{\phi} \,|\, \boldsymbol{\psi}) = \sum_{j=1}^{N} \bar{\phi}_j \psi_j, \tag{B.2}$$

where ϕ_j (ψ_j) denotes the j-th component of the vector $\boldsymbol{\phi}$ ($\boldsymbol{\psi}$). Then the vector space $\boldsymbol{V}$ is found to be an N dimensional Hilbert space. Here, the bar denotes the complex conjugate.

An eigenvector $\boldsymbol{\varphi}$ of the matrix $\mathcal{A}$ is defined by a nonzero element of $\boldsymbol{V}$ which satisfies

$$\mathcal{A}\boldsymbol{\varphi} = \lambda\boldsymbol{\varphi}, \tag{B.3}$$

where $\lambda \in \mathbb{C}$ is called the eigenvalue. Then, the zero vector and the totality of $\boldsymbol{\varphi}$, which belong to the eigenvector corresponding to the eigenvalue λ, are denoted as $\boldsymbol{W}$. This constitutes the $\mathcal{A}$-invariant subspace of $\boldsymbol{V}$. Here $\boldsymbol{W}$ is called an eigenspace corresponding to the eigenvalue λ.

Adjoint matrix $\mathcal{A}^*$ is a matrix which satisfies

$$(\mathcal{A}^*\boldsymbol{\phi} \,|\, \boldsymbol{\psi}) = (\boldsymbol{\phi} \,|\, \mathcal{A}\boldsymbol{\psi}), \tag{B.4}$$

for any $\boldsymbol{\phi}, \boldsymbol{\psi} \in \boldsymbol{V}$. The $\mathcal{A}^*$ is represented by the complex conjugate of the transposed matrix. Hermitian (selfadjoint) matrix is the one which satisfies $\mathcal{A}^* = \mathcal{A}$. It is readily shown that all eigenvalues of the Hermitian matrix are real.[1] Moreover, it is known that all eigenvectors can be taken orthogonal and the totality of eigenspaces span the original vector space:

$$\boldsymbol{V} = \boldsymbol{W}_1 \oplus \boldsymbol{W}_2 \oplus \cdots \oplus \boldsymbol{W}_N, \tag{B.5}$$

where $\oplus$ denotes the direct orthogonal sum of the eigenspaces. It is noted that normal matrices also allow the orthogonal decomposition of the vector space $\boldsymbol{V}$ by their eigenvectors, however, the semi-simple matrices allow the decomposition

$$\boldsymbol{V} = \boldsymbol{W}_1 \dotplus \boldsymbol{W}_2 \dotplus \cdots \dotplus \boldsymbol{W}_N, \tag{B.6}$$

where $\dotplus$ denotes the simple direct sum in which eigenspaces may not be orthogonal.

The spectral resolution of the Hermitian matrix $\mathcal{A}$ will be described with use of the commutability with its adjoint.[2] Let $\mathcal{P}_n$ be the projection operator from $\boldsymbol{V}$ onto $\boldsymbol{W}_n$, then it will be expressed as

$$\mathcal{P}_n = \boldsymbol{\varphi}_n(\boldsymbol{\varphi}_n| \cdot), \tag{B.7}$$

where $\boldsymbol{\varphi}_n \in \boldsymbol{V}$ denotes the normalized eigenvector of the operator $\mathcal{A}$ which corresponds to the eigenvalue λ_n. Here the dimension of the eigenspace $\boldsymbol{W}_n$ is assumed as unity for simplicity. It is noted that Eq. (B.7) is sometimes expressed as $\mathcal{P}_n = |\boldsymbol{\varphi}_n)(\boldsymbol{\varphi}_n|$ in the quantum mechanics context by following Dirac [8]. It is shown that any Hermitian operator $\mathcal{A}$ will be expressed in terms of the projector as

$$\mathcal{A} = \sum_{n=1}^{N} \lambda_n \mathcal{P}_n, \tag{B.8}$$

[1] For any eigenvalue λ and the corresponding eigenvector φ, $(\varphi \,|\, \mathcal{A}\varphi) = \lambda(\varphi \,|\, \varphi)$ holds. On the other hand, $(\varphi \,|\, \mathcal{A}\varphi) = (\mathcal{A}\varphi \,|\, \varphi) = \bar{\lambda}(\varphi \,|\, \varphi)$ also holds, which supports $\lambda = \bar{\lambda}$.

[2] Therefore, the following orthogonal spectral resolution is applicable to more general normal matrix which satisfies $\mathcal{A}^*\mathcal{A} = \mathcal{A}\mathcal{A}^*$.

which is called a spectral resolution of the Hermitian matrix operator $\mathcal{A}$. Here the resolution of identity can be produced as

$$\sum_{n=1}^{N} \mathcal{P}_n = \mathcal{I}, \tag{B.9}$$

where $\mathcal{I}$ denotes the identity matrix, and the orthogonality of the projector

$$\mathcal{P}_i \mathcal{P}_j = 0 \quad (i \neq j) \tag{B.10}$$

holds due to the orthogonality of the eigenvectors.

Based on the above knowledges, we can solve Eq. (B.1) by means of spectral resolution method. Substituting the spectral resolution (B.8) into original Schrödinger type equation (B.1) leads to

$$\begin{aligned} \mathrm{i}\partial_t \boldsymbol{\psi} &= \sum_{n=1}^{N} \lambda_n \mathcal{P}_n \boldsymbol{\psi} \\ &= \sum_{n=1}^{N} \lambda_n \boldsymbol{\varphi}_n (\boldsymbol{\varphi}_n \,|\, \boldsymbol{\psi}). \end{aligned} \tag{B.11}$$

Taking the scalar product of both sides with $\boldsymbol{\varphi}_i$ $(i \in \mathbb{N})$ gives

$$\mathrm{i}\partial_t (\boldsymbol{\varphi}_i |\, \boldsymbol{\psi}) = \lambda_i (\boldsymbol{\varphi}_i |\, \boldsymbol{\psi}), \tag{B.12}$$

due to the orthogonality of eigenvectors. Equation (B.12) is readily solved and we obtain the time evolution of each 'mode' as

$$(\boldsymbol{\varphi}_i |\, \boldsymbol{\psi})(t) = e^{-\mathrm{i}\lambda_i t} (\boldsymbol{\varphi}_i |\, \boldsymbol{\psi})(0) \tag{B.13}$$

Substituting it into resolution of $\boldsymbol{\psi}(t)$

$$\begin{aligned} \boldsymbol{\psi}(t) &= \sum_{n=1}^{N} \mathcal{P}_n \boldsymbol{\psi}(t) \\ &= \sum_{n=1}^{N} \boldsymbol{\varphi}_n (\boldsymbol{\varphi}_n |\, \boldsymbol{\psi})(t), \end{aligned} \tag{B.14}$$

we obtain the general solution as

$$\boldsymbol{\psi}(t) = \sum_{n=1}^{N} \boldsymbol{\varphi}_n e^{-\mathrm{i}\lambda_i t} (\boldsymbol{\varphi}_i |\, \boldsymbol{\psi})(0). \tag{B.15}$$

Since the whole linear vector space $\boldsymbol{V}$ is spanned by only eigenfunctions with real eigenvalues for the Hermitian matrix $\mathcal{A}$, the time evolution is written in the form of the superposition of simple harmonic oscillators (eigenmodes).

It is noted that, up to semi-simple matrix, this method works with slight modifications. The time evolution of the whole system is determined by the exponential function with eigenvalues of the operator as its exponent, even though the orthogonality of eigenmodes may not follow in the case of semi-simple matrix.

B.1.2 Algebraic instability of Jordan matrices

In this section, the pathology of applying the spectral resolution for Jordan matrices is shown. We will invoke here a different method from the previous section. Since finite dimensional matrix operator is a bounded one, we can define the exponential function of the operator as

$$e^{\mathcal{A}} = \mathcal{I} + \mathcal{A} + \frac{1}{2!}\mathcal{A}^2 + \cdots, \tag{B.16}$$

where $\mathcal{I}$ denotes the identity matrix. It is shown that this expression gives a convergent series. Using the exponential function of the matrix, we can write the solution of the original Schrödinger equation (B.1) as

$$\boldsymbol{\psi}(t) = e^{-\mathrm{i}t\mathcal{A}}\boldsymbol{\psi}(0). \tag{B.17}$$

If $\mathcal{A}$ were a Hermitian (semi-simple) matrix, the linear space $\boldsymbol{V}$ would be spanned by eigenvectors. Therefore, the expansion

$$\begin{aligned} e^{-\mathrm{i}t\mathcal{A}} &= e^{-\mathrm{i}\lambda t}e^{-\mathrm{i}t(\mathcal{A}-\lambda\mathcal{I})} \\ &= e^{-\mathrm{i}\lambda t}\Big[\mathcal{I} - \mathrm{i}t(\mathcal{A}-\lambda\mathcal{I}) - \frac{t^2}{2}(\mathcal{A}-\lambda\mathcal{I})^2 + \cdots\Big], \end{aligned} \tag{B.18}$$

applied for the component of the eigenspace corresponding to the eigenvalue λ, would give no contribution except for the first term in the square bracket. It made the problem possible to represent the whole dynamics of the system by the superposition of exponential time evolution.

However, the eigenvectors are not enough, in general, to span the whole linear space $\boldsymbol{V}$ for the Jordan matrix. Let $\boldsymbol{\varphi}$ be one of eigenvectors in a wider sense belonging to the eigenvalue λ, and $(\mathcal{A}-\lambda\mathcal{I})^n\boldsymbol{\varphi}$ vanishes at first for $n \in \mathbb{N}$ $(n > 1)$. That is shown as

$$(\mathcal{A}-\lambda\mathcal{I})^j\boldsymbol{\varphi}\begin{cases} \neq 0 & \text{for} \quad j < n \\ = 0 & \text{for} \quad j \geq n \end{cases}. \tag{B.19}$$

Suppose that the initial condition is taken as $\boldsymbol{\varphi}$. From the expressions shown in Eqs. (B.17) and (B.18), we have

$$\begin{aligned} \boldsymbol{\psi}(t) &= e^{-\mathrm{i}\lambda t}e^{-\mathrm{i}t(\mathcal{A}-\lambda\mathcal{I})}\boldsymbol{\varphi} \\ &= e^{-\mathrm{i}\lambda t}\sum_{j=0}^{n-1}\frac{(-\mathrm{i}t)^j}{j!}(\mathcal{A}-\lambda\mathcal{I})^j\boldsymbol{\varphi}. \end{aligned}$$

Thus, the fastest growing mode of the eigenvector in a wider sense belonging to the eigenvalue λ shows divergence of the dependence $t^{(n-1)}e^{-\mathrm{i}\lambda t}$, which corresponds to an instability even if the eigenvalue λ is real. The algebraic growth of amplitudes is called 'secularity.'

B.2 Differential operator

In this section, we will show an example of spectral resolution for the differential operator corresponding to Schrödinger equation, and compare two widely used methods for the spectral analysis, i.e. Fourier transformation and Laplace transformation. Difficulties of constructing the complete spectral theory for differential operators are coming from the infinity of their dimensions, which leads to the appearance of continuous spectra, and unboundedness of their spectra. However, we will not discuss such difficulties in this section. For readers who are interested in such profound problems, several mathematical books are useful [28, 11, 6]. It is also noted that the following discussions may not follow with the terminology of modern mathematics.

B.2.1 Spectral resolution

First, we will consider the one dimensional Laplacian operator

$$\mathcal{A} = \partial_x^2, \tag{B.20}$$

defined in the Sobolev space $H_0^1[0,1]$. Here, $H_0^1[0,1]$ denotes the set of the once differentiable functions $f(x)$ defined in the region $x \in [0,1]$ which satisfies the boundary condition $f(0) = f(1) = 0$. The scalar product in this functional space is defined by

$$(u \,|\, v) = \int_0^1 \bar{u} v \, \mathrm{d}x, \tag{B.21}$$

for the elements $u, v \in H_0^1[0,1]$, where the bar denotes the complex conjugate. It is readily shown that the operator $\mathcal{A}$ is Hermitian (selfadjoint) in this functional space.

Since

$$\frac{\mathrm{d}^2}{\mathrm{d}x^2} \sin(n\pi x) = -(n\pi)^2 \sin(n\pi x) \tag{B.22}$$

holds, the eigenvalues of the operator $\mathcal{A}$ are

$$\lambda_n = -(n\pi)^2 \quad (n \in \mathbb{N}), \tag{B.23}$$

and the corresponding normalized eigenfunctions are

$$u_n = \sqrt{2} \sin(n\pi x). \tag{B.24}$$

It is known that this set of eigenfunctions u_n constitutes a complete orthogonal basis in $H_0^1[0,1]$ with the scalar product (B.21). Therefore, an arbitrary function $\phi \in H_0^1[0,1]$ will be expanded as

$$\phi(x) = \sum_{n=1}^{\infty} a_n u_n(x), \tag{B.25}$$

where a_n is given by

$$a_n = (u_n \,|\, \phi). \tag{B.26}$$

It is noted here that the operator

$$\mathcal{P}_n = |u_n)(u_n| = u_n(x) \int_0^1 u_n(x) \;\cdot\; \mathrm{d}x \tag{B.27}$$

describes the projection from $H_0^1[0,1]$ onto the subspace spanned by $|u_n)$ and the spectral resolution of $\mathcal{A}$ is denoted as

$$\mathcal{A} = \sum_{n=1}^{\infty} \lambda_n \mathcal{P}_n, \tag{B.28}$$

which shows the formal equivalence between the matrix representation and the differential one in quantum mechanics [8, 22]. Furthermore,

$$\sum_{n=1}^{\infty} \mathcal{P}_n = 1 \tag{B.29}$$

is called the resolution of identity for the operator $\mathcal{A}$, which is obtained from the Parseval's equality

$$\|\phi\|^2 = \sum_{n=1}^{\infty} |(u_n \,|\, \phi)|^2, \tag{B.30}$$

where $\|\phi\| = (\phi \,|\, \phi)$ denotes the norm of the element ϕ. The possibility of constructing the resolution of identity by means of eigenfunctions is guaranteed only for Hermitian operators (von Neumann theorem). Although this resolution is not always expressed by the summation — in general, the Hermitian operator of the Hilbert space contains the continuous spectra, we have taken such a space for simplicity. In the extension of the previous sections, it is quite natural to consider that non-Hermitian operators may include eigenfunctions in a wider sense.

Based on the above knowledges, we can solve the following time evolution equation (Schrödinger equation for a free particle);

$$\mathrm{i}\partial_t \psi = \partial_x^2 \psi, \tag{B.31}$$

by means of the spectral resolution of the operator $\mathcal{A}$. Expanding ψ by the eigenfunctions u_n of the operator $\mathcal{A}$ as

$$\psi(x,t) = \sum_{n=1}^{\infty} a_n(t) u_n(x), \tag{B.32}$$

and substituting it into Eq. (B.31), we have

$$\sum_{n=1}^{\infty} (\mathrm{i}\partial_t a_n - \lambda_n a_n) u_n = 0. \tag{B.33}$$

Since u_n is orthogonal for different n, the equation can be decomposed into the one for each 'mode' to give

$$\mathrm{i}\partial_t a_n = \lambda_n a_n, \tag{B.34}$$

which leads to the solution of each mode as

$$a_n(t) = a_n(0) e^{-\mathrm{i}\lambda_n t}. \tag{B.35}$$

Thus, the general solution for an arbitrary initial perturbation $\psi(x, 0)$ can be obtained as

$$\psi(x,t) = \sum_{n=1}^{\infty} \sqrt{2} a_n(0) e^{\mathrm{i}n^2\pi^2 t} \sin(n\pi x), \tag{B.36}$$

where $a_n(0)$ is obtained by

$$a_n(0) = (u_n \,|\, \psi(x, 0)). \tag{B.37}$$

B.2.2 Fourier transformation

Let us solve the Schrödinger equation (B.31) by means of the Fourier transformation. This method is intrinsically parallel to the spectral resolution.

Fourier transformation is formally defined as

$$\hat{\psi}(k,\omega) = \int_0^1 \int_{-\infty}^{\infty} \psi(x,t)\, e^{-\mathrm{i}(kx-\omega t)}\, \mathrm{d}t\, \mathrm{d}x, \tag{B.38}$$

where the inversion will be given by

$$\psi(x,t) = \frac{1}{2\pi} \sum_k \int_{-\infty}^{\infty} \hat{\psi}(k,\omega)\, e^{\mathrm{i}(kx-\omega t)}\, \mathrm{d}\omega, \tag{B.39}$$

where the inversion with respect to k is expressed by the discrete summation since we have taken the finite domain [0,1]. The wave number k is chosen as

$$k = n\pi \quad (n \in \mathbb{N}). \tag{B.40}$$

We will apply the Fourier transformation to the Schrödinger equation and obtain

$$(\omega + k^2)\hat{\psi}(k,\omega) = 0, \tag{B.41}$$

which is readily solved for $\hat{\psi}$ to give

$$\hat{\psi}(k,\omega) = \delta(\omega + k^2). \tag{B.42}$$

The relation

$$\omega = -k^2, \tag{B.43}$$

denoting the singularity of $\hat{\psi}$, is called the 'dispersion relation' since only these values which satisfy Eq. (B.43) will give the contribution when inverted.

The way of solving the initial value problem is described as follows. Since an initial perturbation can be spatially Fourier transformed as

$$\hat{a}(k) = \int_0^1 \psi(x,0)\, e^{-\mathrm{i}kx}\, \mathrm{d}x, \tag{B.44}$$

the solution will be given by the superposition of singular eigenfunction $\hat{\psi}(k,\omega)$ multiplied by $\hat{a}(k)$, which leads to

$$\begin{aligned}\psi(x,t) &= \sum_k \int_{\infty}^{-\infty} \hat{a}(k)\delta(\omega + k^2)\, e^{\mathrm{i}(kx-\omega t)}\, \mathrm{d}\omega \\ &= \sum_{n=1}^{\infty} \hat{a}_n \exp[\mathrm{i}(n\pi x + n^2\pi^2 t)],\end{aligned} \tag{B.45}$$

where we have defined $\hat{a}_n = \hat{a}(k)$ with the relation (B.40). This expression exactly coincides with the solution obtained by the spectral resolution (B.36) by taking the real part of Eq. (B.45).

It should be noted that the Fourier transformation in time corresponds to the expression with whole superposition *on* the spectra, which now has a discrete sum of projections onto point eigenvalues.

B.2.3 Laplace transformation

Here we will solve the same Schrödinger equation (B.31) with an another method, i.e. Fourier transformation in space and Laplace transformation in time.

Fourier-Laplace transformation of the perturbed field is defined as

$$\tilde{\psi}(k,s) = \int_0^1 \int_0^{\infty} \psi(x,t)\, e^{-\mathrm{i}kx-st}\, \mathrm{d}t\, \mathrm{d}x, \tag{B.46}$$

where the real part of s is chosen to be larger than any temporal singularity of the function $\psi(t)$ for the convergence of the integration. The inversion will be given by

$$\psi(x,t) = \frac{1}{2\pi\mathrm{i}} \sum_k \int_{s_0-\mathrm{i}\infty}^{s_0+\mathrm{i}\infty} \tilde{\psi}(k,s)\, e^{\mathrm{i}kx+st}\, \mathrm{d}s, \tag{B.47}$$

where $s_0 = \mathrm{Re}(s) > 0$ and k satisfies the condition (B.40).

The Fourier-Laplace transformation of the Schrödinger equation (B.31) gives

$$\mathrm{i}s\tilde{\psi} = -k^2\tilde{\psi} + \mathrm{i}\bar{\psi}(k,0), \tag{B.48}$$

which leads to

$$\tilde{\psi}(k,s) = \frac{\bar{\psi}(k,0)}{s - \mathrm{i}k^2}. \tag{B.49}$$

Here $\bar{\psi}(k,0)$ denotes the spatially Fourier transformed initial value

$$\bar{\psi}(k,0) = \int_0^1 \psi(x,0)\, e^{-\mathrm{i}kx}\, \mathrm{d}x. \tag{B.50}$$

By inverting Eq. (B.49), we obtain

$$\begin{aligned} \psi(x,t) &= \frac{1}{2\pi \mathrm{i}} \sum_k \int_{s_0 - \mathrm{i}\infty}^{s_0 + \mathrm{i}\infty} \frac{\bar{\psi}(k,0)}{s - \mathrm{i}k^2}\, e^{\mathrm{i}kx + st}\, \mathrm{d}s, \\ &= \sum_{n=1}^{\infty} \bar{\psi}(k,0)\, \exp[\mathrm{i}(n\pi x + n^2\pi^2 t)], \end{aligned} \tag{B.51}$$

which again coincides with the previous two methods.

It is noted that the Laplace transformation method in time corresponds to the expression with whole integration *around* the spectra, which is now rewritten by the discrete sum of independent eigenmodes due to Cauchy's integral theorem.