A THEORETICAL AND NUMERICAL STUDY FOR THE FOKKER-PLANCK EQUATION

by

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Abstract

In this thesis, the Fokker-Planck equation is investigated theoretically and numerically. A class of tridiagonal matrices related to the static solution of the Fokker-Planck equation is also considered. The first part of the thesis is devoted to the existence of solutions to the one dimensional Fokker-Planck equation. The existence is proved using semigroup theory. In the second part, the spectral method using Hermite functions is developed for the one dimensional Fokker-Planck equation. Numerical results are also presented. The third part of the thesis is to extend the Hermite spectral method to the two dimensional equation. The last part is concerned with the distribution of eigenvalues for certain tridiagonal matrices. We prove that all eigenvalues of these matrices lie on the left half plane. This property is crucial for the spectral approximation to the static solution of the Fokker-Planck equation.

Dedication

TO: LEIWEN

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Chapter 1

Introduction

Fluctuations are a very common feature in a large number of fields. Nearly every system is subjected to complicated external or internal influences that are not fully known and that are often termed noise or fluctuations. The Fokker-Planck equation deals with those fluctuations of systems which stem from many tiny disturbances, each of which changes the variables of the system in an unpredictable but small way. The Fokker-Planck equation was first applied to the Brownian motion problem (see, e.g. [8, 22]). Here the system is a small but macroscopic particle, immersed in fluid. The molecules of the fluid kick around the particle in an unpredictable way so the position of the particle fluctuates. Because of these fluctuations we do not know its position exactly, but instead we have a certain probability to find the particle in a given region. With the Fokker-Planck equation such a probability density can be determined. This equation is now used in a number of different fields in natural science, for instance in solid-state physics, quantum optics, chemical physics, theoretical biology and circuit theory.

One of the simplest Fokker-Planck equations is

$$\frac{\partial W}{\partial t} = \gamma \frac{\partial (vW)}{\partial v} + \gamma \beta \frac{\partial^2 W}{\partial v^2}, \qquad (1.1)$$

where W(v,t) is the distribution function, γ^{-1} the particle relaxation time, $\beta = kT/m$

is the thermal velocity, k is the Boltzmann's constant, T the temperature and m the mass of particle. By solving (1.1) starting with W(v, 0) and subject to the appropriate boundary conditions, one may obtain the distribution function W(v,t) for all later times. In general, the distribution function W depends not only on velocity but also on position. For example, Kramer's equation is an equation of motion for distribution functions in position and velocity space describing the Brownian motion of particles in an external field. For details of the Fokker-Planck equations the reader is referred to [22].

Solutions (esp. the stationary solutions) of the Fokker-Planck equation often decay at infinity at least like $\exp(-pv^2)$ for some positive constants p (i.e. Gaussian type). Therefore, the Hermite expansions have natural applications for the Fokker-Planck equation. The normalized Hermite functions are

$$\psi_n(v) = \frac{1}{\sqrt{2^n n!}} H_n(v) \exp\left(-\frac{v^2}{2}\right),$$
(1.2)

where the $H_n(v)$ are the usual (unnormalized) Hermite polynomials. Many researchers have noticed that the close connection of Hermite functions to the physics makes them a natural choice of basis functions for many fields of science and engineering, (see for example Chapter 14 of [5] and the introduction of [25]). Also one of the reasons for using Hermite spectral methods is that the Hermite system has some very attractive properties from the numerical point of view (see, e.g. [4, 13, 28]). It is shown in [28] that the spectral radii for the first and second Hermite differentiation matrices are $O(\sqrt{N})$ and O(N), respectively, where N + 1 is the number of truncated terms used. This places rather weak stability restrictions on the Hermite method. For example, if we consider the standard heat equation, then a maximum step size in the time direction of order $O(N^{-1})$ is required, whereas for Fourier and Chebyshev methods it is of order $O(N^{-2})$ and $O(N^{-4})$, respectively. In the actual calculations this means that one need not even consider implicit time integration methods with the Hermite method.

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In this thesis, we shall study the theoretical properties of the Fokker-Planck equation. Numerical methods based on the Hermite expansion will be also investigated. The first part of this thesis is devoted to the existence of solutions for the one dimensional Fokker-Planck equation. We shall employ the semigroup theory to prove the existence property for the one-dimension Fokker-Planck equation. There has been a number of papers dealing with the existence of the solutions for various equations including the Fokker-Planck equation (see, e.g. [20, 12]), but none of these has used the semigroup theory. In the second part, a spectral method using Hermite functions is developed for the one dimensional Fokker-Planck equation. The ordinary differential equation system derived from this method shows a very good simulation to the Fokker-Planck equation. This can be seen from both the theoretical analysis and the numerical examples. The trapezoidal method is used to solve the ordinary differential equation system. In the third part, we apply the spectral method developed in [26] to the two dimensional Fokker-Planck equation. The coefficients matrix involved in the partial differential equation system derived from this method shows that the partial differential equation system is hyperbolic. Artificial boundaries are set up for this PDE system since the domain of the space variable is unbounded.

In the last part of this thesis, we consider the eigenvalues of a class of tridiagonal matrices, which will appear when the Hermite spectral method is applied to the one dimensional Fokker-Planck equation in the more general case. Each matrix in this class cannot be similarly transformed into a symmetric matrix and may have complex eigenvalues. We prove that all the eigenvalues of such a matrix lie on one of the half planes depending on the signs of the diagonal entries. This property is very important in showing that the solutions of an ordinary differential equation system with such a matrix are decaying. Some examples are given in this part to show some further properties of this class of matrices.

Chapter 2

The existence of the solution

In this chapter, a model 1-D Fokker-Planck equation is investigated. The equation is given by

$$\frac{\partial u}{\partial t} = \frac{\partial (xu)}{\partial x} + \frac{\partial^2 u}{\partial x^2} - \infty < x < +\infty$$
(2.1)

together with an initial condition

$$u(0) = u_0. (2.2)$$

The solution of Eqs. (2.1) and (2.2) is required to satisfy

$$\int_{-\infty}^{+\infty} u(x)dx = \int_{-\infty}^{+\infty} u_0(x)dx.$$
 (2.3)

The Eq. $(2.3 \text{ is a natural property of the solution, i.e. the conservation of the mass, and will be discussed later. The semigroup method is used to prove the existence of a solution to this equation.$

In the following sections, we introduce some useful results from semigroup theory, which can be found in [19, 30]. Throughout this chapter the letter C will denote a generic constant whose meaning and value varies with context.

2.1 Semigroup and its application to evolution equations

In this section some concepts of semigroups and major results related to the applications in this chapter will be briefly described.

Definition 2.1 Let X be a Banach space. A one parameter family T(t), $0 \le t < \infty$, of bounded linear operators from X into X is said to be a semigroup of bounded linear operators on X if

(i) T(0) = I, (I is the identity operator on X); (ii) T(t+s) = T(t)T(s) for every $t, s \ge 0$ (the semigroup property).

A semigroup of bounded linear operators, T(t), is uniformly continuous if

$$\lim_{t \downarrow 0} \| T(t) - I \| = 0.$$
(2.4)

The linear operator A defined by

$$Ax = \lim_{t \downarrow 0} \frac{T(t)x - x}{t} \quad \text{for} \quad x \in D(A),$$
(2.5)

where D(A) is a set defined by

$$D(A) = \{x \in X : \lim_{t \downarrow 0} \frac{T(t)x - x}{t} \quad \text{exists}\},$$
(2.6)

is the infinitesimal generator of the semigroup T(t), with D(A) being the domain of A.

Definition 2.2 A semigroup $T(t), 0 \le t < \infty$, of bounded linear operators on X is a strongly continuous semigroup of bounded linear operators if

$$\lim_{t \downarrow 0} T(t)x = x \quad \forall x \in X.$$
(2.7)

A strongly continuous semigroup of bounded linear operators on X will be called a semigroup of class C_0 or simply a C_0 -semigroup.

Definition 2.3 Let T(t) be a C_0 -semigroup. T(t) is called a C_0 -semigroup of contractions if

$$|| T(t) || \le 1 \quad \forall t \ge 0$$
 (2.8)

With these definitions, we have the following lemmas:

Lemma 2.1 (Hille-Yosida) (See, e.g., [19]) A linear (unbounded) operator A is the infinitesimal generator of a C_0 -semigroup of contractions $T(t), t \ge 0$ if and only if

(i) D(A) is dense in X, i.e., $\overline{D(A)} = X$; (ii) Let $J_{\lambda} = (I - \lambda A)^{-1}$ for $\lambda > 0$, then

 $\| J_{\lambda} \|_{\mathcal{L}(X,X)} \le 1 \quad \forall \lambda > 0.$ (2.9)

Consider the following abstract Cauchy problem:

$$\frac{du(t)}{dt} = Au(t) \tag{2.10}$$

and

$$u(0) = x \in X \tag{2.11}$$

where X is a Banach space and A is a linear operator from $D(A) \subset X$ into X. Then we have:

Lemma 2.2 (See, e.g., [19]) If A is an infinitesimal generator of a C_0 -semigroup of contractions T(t), then for every $u_0 \in D(A)$ the Cauchy problem has a unique solution $u \in C^1([0,\infty), X) \cap C^0([0,\infty), D(A)).$

Now we consider the inhomogeneous Cauchy problem:

$$\frac{du(t)}{dt} = Au(t) + F(u) \quad \forall t > 0$$
(2.12)

with

$$u(0) = x \in X \tag{2.13}$$

We have the following lemma about the solution of inhomogeneous Cauchy problems Lemma 2.3 (See, e.g., [19]) In addition to the hypotheses in the above lemma, let F be Lipschitz continuous from X to X, i.e., there exists a constant L such that:

$$|| F(u) - F(v) || \le L || u - v ||$$
 for any $u, v \in X$ (2.14)

and $F \in C^1(X,X), u_0 \in D(A)$. Then the inhomogeneous Cauchy problem has a unique solution $u \in C^1([0,\infty), X) \cap C^0([0,\infty), D(A))$.

2.2 The existence of the 1–D Fokker–Planck equation

Now we turn to the 1-D Fokker-Planck equation:

$$\frac{\partial u}{\partial t} = \frac{\partial (xu)}{\partial x} + \frac{\partial^2 u}{\partial x^2} \quad -\infty < x < \infty \tag{2.15}$$

with

 $u(0) = u_0,$ (2.16)

$$\frac{\partial u}{\partial t} = x \frac{\partial u}{\partial x} + \frac{\partial^2 u}{\partial x^2} + u$$
(2.17)

with

$$u(0) = u_0. (2.18)$$

Let

 $X = L^2(R)$

and

$$D(A) = \{u \mid u, u', xu', u'' \in L^{2}(R)\}.$$

Let A, F be the two operators defined by

4

$$Au = xu' + u'' \tag{2.19}$$

and

$$Fu = u. \tag{2.20}$$

The above problem (2.17) and (2.18) can be written as the following Cauchy problem:

$$\frac{du(t)}{dt} = Au(t) + Fu(t), \quad \text{for} \quad t > 0$$
(2.21)

with

$$u(0) = u_0 \in X. \tag{2.22}$$

We will prove

 $|| J_{\lambda} || \leq 1 \quad \forall \lambda > 0,$

or equivalently,

 $|| u_{\lambda} || \leq || f || \quad \forall \lambda > 0,$

where u_{λ} is the solution of the following equation:

 $u - \lambda(xu' + u'') = f.$ (2.23)

Consider the following variational problem associated with the above equation: Find $u \in H_1$, such that

$$a_{\lambda}(u,v) = f(v) \quad \forall v \in H_2, \tag{2.24}$$

where $H_2 = H^1(R) = \{u | u, u' \in L^2\}, H_1 = \{u | u \in H^1(R), xu' \in L^2\}, f \in H'_2$, the dual space of H_2 , and $a_{\lambda}(u, v)$ is a bilinear form over $H_2 \times H_1$ defined by

$$a_{\lambda}(u,v) = \int_{-\infty}^{+\infty} (uv - \lambda x u'v + \lambda u'v') dx. \qquad (2.25)$$

For simplicity, we will drop subscript λ . Thus we have

Theorem 2.1 If there is a $v_0 \in H_1$ such that

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$$a(u, v_0) = 0 \quad \forall u \in H_2, \tag{2.26}$$

then $v_0 = 0$.

Proof. Let φ_n be defined by

$$\varphi_n(t) = (2^n n! \sqrt{\pi})^{-\frac{1}{2}} e^{-\frac{t^2}{2}} H_n \tag{2.27}$$

for $n = 0, 1, 2, \cdots$. Then we know that the set $\varphi_n, n = 0, 1, 2, \cdots$ is a complete orthonormal basis in $L^2(R)$, where H_n is the Hermite polynomial of degree n. So v_0 has a unique expansion in terms of φ_n :

$$v_0 = \sum_{n=0}^{\infty} c_n \varphi_n \tag{2.28}$$

where $c_n = \int_{-\infty}^{+\infty} v_0 \varphi_n$. For $\varphi_n, n = 1, 2, 3, \ldots$, we have

$$\varphi'_{n} = \sqrt{\frac{n}{2}}\varphi_{n-1} - \sqrt{\frac{n+1}{2}}\varphi_{n+1},$$
 (2.29)

$$x\varphi'_{n} = \sqrt{\frac{n(n-1)}{2}}\varphi_{n-2} - \frac{1}{2}\varphi_{n} - \sqrt{\frac{(n+1)(n+2)}{2}}\varphi_{n+2}$$
(2.30)

and

$$v_0' = \sum_{n=0}^{+\infty} d_n \varphi_n. \tag{2.31}$$

where

$$d_n = \sqrt{\frac{n+1}{2}} c_{n+1} - \sqrt{\frac{n}{2}} c_{n-1}$$
 (2.32)

and

$$\varphi_{-2} = \varphi_{-1} = c_{-1} = c_{-2} = 0. \tag{2.33}$$

If we choose $u = \varphi_n$, then

$$a(u,v) = c_n - \frac{\lambda}{2} \left[\sqrt{(n(n-1))} c_{n-2} - c_n - \sqrt{((n+1)(n+2))} c_{n+2} \right] + \lambda \left[\sqrt{\frac{n}{2}} d_{n-1} - \sqrt{\frac{n+1}{2}} d_{n+1} \right] = c_n - \lambda (n(n-1))^{1/2} c_{n-2} + \lambda (n+1) c_n = 0.$$
(2.34)

Therefore

$$c_n = \frac{\lambda (n(n-1))^{1/2}}{1 + \lambda (1+n)} c_{n-2}.$$
 (2.35)

One easily sees that $c_0 = c_1 = 0$. Hence by using the recursive formula (2.35) we deduce that

$$c_n = 0$$
 for $n = 1, 2, 3, \cdots$ (2.36)

This completes the proof. \Box

Theorem 2.2 $a(u,u) \geq C \parallel u \parallel^2_{H_2} \quad \forall u \in H_1 \subset H_2$

12.

Proof. Using integration by parts we have

$$\int_{-\infty}^{+\infty} xu'udx = -\int_{-\infty}^{+\infty} u(xu)'dx$$
$$= -\int_{-\infty}^{+\infty} u^2dx - \int_{-\infty}^{+\infty} xu'udx \qquad (2.37)$$

so that

$$\int_{-\infty}^{+\infty} x u' u dx = -\frac{1}{2} \int_{-\infty}^{+\infty} u^2 dx.$$
 (2.38)

Therefore

$$a(u,u) = \int_{-\infty}^{+\infty} u^2 dx - \lambda \int_{-\infty}^{+\infty} x u' u dx + \lambda \int_{-\infty}^{+\infty} (u')^2 dx$$

$$= \int_{-\infty}^{+\infty} u^2 dx + \frac{\lambda}{2} \int_{-\infty}^{+\infty} u^2 dx + \lambda \int_{-\infty}^{+\infty} (u')^2 dx$$

$$\geq C \parallel u \parallel_{H_2}^2 \quad \forall u \in H_1$$
(2.39)

where $c = \frac{\lambda}{2} > 0$. \Box

The proof of the following theorem for the variational problem (2.24) is similar to that of the Lax-Milgram lemma (See, e.g., [9]).

Theorem 2.3 Assume the bilinear form a(u, v) is defined by (2.25) and $f \in H'_2$. Then there is a unique solution to the variation problem (2.24). **Proof.** Obviously, $a(\cdot, \cdot)$ is a bilinear form on $H_1 \times H_2$. Then for a fixed $u \in H_1, a(u, \cdot)$ is a linear functional on H_2 . Since H_2 is a Hilbert space, by the Riesz representation theorem, there is an element $R(u) \in H_2$ such that

$$a(u,v) = (R(u),v)_{H_2}$$
(2.40)

where (\cdot, \cdot) represents the inner product on H_2 . Assuming $R(u_n), n = 1, 2, 3, ...$ is a Cauchy sequence in H_2 , then $(R(u_n), v), n = 1, 2, 3, ...$ is a bounded set of real numbers for every $v \in H_2$. On the other hand, we may think of $(R(u_n), v)$ as a linear functional on H_1 for every fixed u_n and denote this by

$$(u_n, w) = (u_n, G(v)) \quad \forall v \in H_2.$$

$$(2.41)$$

Then $(u_n, w), n = 1, 2, 3, ...$ is bounded for every $w \in H_1$. Therefore by the resonance theorem, $||u_n||, n = 1, 2, 3, ...$ is bounded. Since H_1 is a separable Hilbert space, there is a $u^* \in H_1$ such that u_n weakly converges to u^* . Thus

$$\lim_{n \to \infty} (u_n, G(v)) = (u^*, G(v)) \quad \forall v \in H_2,$$
(2.42)

or,

$$\lim_{n \to \infty} (R(u_n), v) = (R(u^*), v) \quad \forall v \in H_2.$$
(2.43)

Since $R(u_n)$, n = 1, 2, 3, ... is a Cauchy sequence, $R(u_n)$ must converge to $R(u^*) \in H_2$. This implies $R(H_1)$ is closed. By Theorem 2.1 we obtain

$$R(H_1) = H_2, (2.44)$$

from which we may conclude the existence of a solution to the variational problem (2.24). The uniqueness can be simply proved by the inequality (2.39). \Box

Now we turn to the question of regularity of solutions of the equation

$$u - \lambda (xu' + u'') = f.$$
 (2.45)

CHAPTER 2. THE EXISTENCE OF THE SOLUTION

If $f \in L^2 \subset H'_2$, we know that there is a solution $u \in H_1$, i.e. $u, xu' \in L^2$, therefore $u'' \in L^2$. Besides, we have

$$\int_{-\infty}^{+\infty} u^2 dx + \frac{\lambda}{2} \int_{-\infty}^{+\infty} u^2 dx + \lambda \int_{-\infty}^{+\infty} (u')^2 dx = \int_{-\infty}^{+\infty} f u dx.$$
(2.46)

So

$$(\int_{-\infty}^{+\infty} u^2 dx)^{1/2} \le (\int_{-\infty}^{+\infty} f^2)^{1/2},$$
(2.47)

which implies that

$$\| (I - \lambda A)^{-1} \|_{\mathcal{L}(X,X)} \le 1 \quad \forall \lambda > 0.$$
 (2.48)

By theorem 2.1, theorem 2.2, theorem 2.3 and all the lemmas in the previous section, we have

Theorem 2.4 Operator A defined by (2.19) is an infinitesimal generator of a C_0 -semigroup of contractions. Therefore, Cauchy problem (2.21) (2.22) has a unique solution $u \in C^1([0,\infty), X) \cap C^0([0,\infty), D(A))$.

Remark 2.1 Some investigation of L^1 theory for the existence of the solution. We will first derive an estimate for $u \in L^1(R)$. Set

$$\psi_n(x) = \left\{ egin{array}{lll} 1 & ext{if } x < -1/n \ nx & ext{if } -1/n < x < 1/n \ 1 & ext{if } x > 1/n \end{array}
ight.$$

Then

$$\lim_{n \to \infty} \int_{-\infty}^{+\infty} u \psi_n(u) dx = \int_{-\infty}^{+\infty} |u| dx$$
 (2.49)

since $\psi_n(u) \to 2\delta(u)$ as $n \to \infty$. Also

$$-\int_{-\infty}^{+\infty} x u' \psi_n(u) dx = \int_{-\infty}^{+\infty} u \psi_n(u) dx + \int_{-\infty}^{+\infty} x u \psi_n(u)' u' dx \qquad (2.50)$$

$$-\int_{-\infty}^{+\infty} u'' \psi_n(x) dx = \int_{-\infty}^{+\infty} \psi_n(u) (u')^2 dx \ge 0.$$
 (2.51)

and

Thus, from

$$\int_{-\infty}^{+\infty} u\psi_n(x)dx - \lambda \int_{-\infty}^{+\infty} xu'\psi_n(x)dx - \lambda \int_{-\infty}^{+\infty} u''\psi_n(x)dx$$
$$= \int_{-\infty}^{+\infty} f\psi_n(x)dx \qquad (2.52)$$

we have

$$\int_{-\infty}^{+\infty} |u| dx \le \int_{-\infty}^{+\infty} |f| dx \quad \text{if } f \in L^1.$$
(2.53)

Now assume $u \in L^1$. Then the equation

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$$u - \lambda x u' - \lambda u'' = f \tag{2.54}$$

may be rewritten as

$$xu' + u'' = g = -(1/\lambda)(f - u), \quad g \in L^1.$$
 (2.55)

Therefore

$$u' = e^{-\frac{x^2}{2}} \int_{-\infty}^{x} e^{\frac{s^2}{2}} g ds.$$
 (2.56)

Note that at large x,

$$u' = \frac{\int_{-\infty}^{x} e^{-\frac{s^2}{2}} g ds}{e^{-\frac{x^2}{2}}} \sim \frac{e^{-\frac{x^2}{2}} g}{x e^{-\frac{x^2}{2}}} = \frac{g}{x}.$$
 (2.57)

So that

 $xu' \sim g$, at large x.

This means $xu' \in L^1$. By using the differential equation we see $u'' \in L^1$. Based on these observations, we deduce that the operator A is also an infinitesimal generator of a C_0 -semigroup of contractions on $X_2 = L^1(R)$, where

$$D(A) = \{ u \mid u, u', xu', u'' \in L^1 \}.$$
 (2.58)

The Cauchy problem has results in L^1 -setting that are similar to those in L^2 -setting.

Remark 2.2 L^1 theory should be more natural. Consider the static solution of the equation, i.e.,

$$(xu)'+u''=0.$$

We have

$$xu + u' = C_1$$

and

$$u = C_1 e^{-\frac{x^2}{2}} \int_{-\infty}^{x} e^{\frac{s^2}{2}} ds + C_2 e^{-\frac{x^2}{2}}.$$

The asymptotic relation

$$\frac{\int_{-\infty}^{x} e^{-\frac{s^2}{2}} ds}{e^{-\frac{x^2}{2}}} \sim \frac{1}{x} \quad \text{at large } x$$

tells us u is in L^2 for any constant C_1 , but not in L^1 unless $C_1 = 0$. On the other hand, formally integrating the Fokker-Planck equation, we have

$$\frac{d\int_{-\infty}^{+\infty} u dx}{dt} = \lim_{x \to \infty} (xu + u') = 0,$$

under the assumption $\lim_{x\to\infty} xu = 0$. Therefore

$$\int_{-\infty}^{+\infty} u dx \equiv \int_{-\infty}^{+\infty} u_0 dx.$$

Therefore, if the solutions are sought in L^2 , then the Fokker-Planck equation may have nonunique static solutions while if the solutions are sought in L^1 , the static solution is unique, determined by the initial data u_0 .

Chapter 3

Spectral method in one dimensional case

In this chapter, the Hermite spectral method is employed for the Fokker-Planck equation. The convergence rate of the spectral method is high for many classes of problems (if the solution is sufficiently smooth) compared to the finite element method or finite difference method. For example, suppose we use a spectral method and a finite difference method to solve two point boundary value problem. If the number of the grid points is N, then the convergence rate of the difference method will not be changed as N grows, but the convergence rate of the spectral method will grow as N grows. The reason for this is: spectral method uses global functions to approximate the solution and the differential equation is usually demanded to be satisfied at a set of points, for example, collocation points. So it is like an N-th order approximation. In many cases the spectral method converges at exponential rate. Because of the high convergence rate the spectral method has become more and more popular, especially after it was found that the FFT technique can be applied to spectral methods (See [4] and [5]). The spectral method for the Fokker-Planck equation will be introduced in sections 3.1 and 3.2. The numerical results will be presented in section 3.3.

3.1 Hermite spectral method

We assume that the solution of the Fokker-Planck equation has the following series expansion:

$$u(x,t) = \sum_{n=0}^{\infty} c_n(t)\varphi_n(x), \qquad (3.1)$$

where

$$\varphi_n = (2^n n! \sqrt{\pi})^{-\frac{1}{2}} e^{-\frac{x^2}{2}} H_n, n = 1, 2, 3, \cdots$$
 (3.2)

in which $H_n(x)$ is the Hermite polynomial of degree *n*. For φ_n defined above, one can find the following recurrence relations:

$$\varphi'_n = (\frac{n}{2})^{1/2} \varphi_{n-1} - (\frac{n+1}{2})^{1/2} \varphi_{n+1},$$
(3.3)

$$x\varphi_n = (\frac{n}{2})^{1/2}\varphi_{n-1} + (\frac{n+1}{2})^{1/2}\varphi_{n+1}, \qquad (3.4)$$

$$x\varphi'_{n} = \frac{(n(n-1))^{1/2}}{2}\varphi_{n-2} - \frac{1}{2}\varphi_{n} - \frac{((n+1)(n+2))^{1/2}}{2}\varphi_{n+2}$$
(3.5)

and

$$\varphi_n'' = \frac{(n(n-1))^{1/2}}{2}\varphi_{n-2} - (n+\frac{1}{2})\varphi_n + \frac{((n+1)(n+2))^{1/2}}{2}\varphi_{n+2}.$$
 (3.6)

By these relations, we have

$$xu_{x} = \sum_{n=0}^{\infty} \frac{(n(n-1))^{1/2}}{2} c_{n} \varphi_{n-2} - \sum_{n=0}^{\infty} \frac{1}{2} c_{n} \varphi_{n}$$

$$- \sum_{n=0}^{\infty} \frac{((n+1)(n+2))^{1/2}}{2} c_{n} \varphi_{n+2}$$

$$= \sum_{n=0}^{\infty} \frac{((n+1)(n+2))^{1/2}}{2} c_{n+2} \varphi_{n} - \sum_{n=0}^{\infty} \frac{1}{2} c_{n} \varphi_{n}$$

$$\sum_{n=0}^{\infty} \frac{(n(n-1))^{1/2}}{2} c_{n-2} \varphi_{n}$$

$$= \sum_{n=0}^{\infty} \left[\frac{((n+1)(n+2))^{1/2}}{2} c_{n+2} - \frac{1}{2} c_{n} - \frac{(n(n-1))^{1/2}}{2} c_{n-2} \right] \varphi_{n}, \quad (3.7)$$

where $c_{-1} = c_{-2} = 0$. Similarly, we have

$$u_{xx} = \sum_{n=0}^{\infty} \left[\frac{((n+1)(n+2))^{1/2}}{2} c_{n+2} - \frac{2n+1}{2} c_n + \frac{(n(n-2))^{1/2}}{2} c_{n-2} \right] \varphi_n. \quad (3.8)$$

By substituting these into the Fokker-Planck equation (2.1) and equating the coefficients of φ_n on the two sides, we have the following ordinary differential system:

$$c'_{n} = -nc_{n} + ((n+1)(n+2))^{1/2}c_{n+2}, \quad n = 0, 1, 2, \cdots$$
 (3.9)

Let $d_k = c_{2k}$, $e_k = c_{2k+1}$, $k = 0, 1, 2, \cdots$. Then, the above equations become

$$d'_{k} = -2kd_{k} + ((2k+1)(2k+2))^{1/2}d_{k+1}$$
(3.10)

and

$$e'_{k} = -(2k+1)e_{k} + ((2k+2)(2k+3))^{1/2}e_{k+1}$$
(3.11)

where $k = 0, 1, 2, \cdots$. Take an approximation of u as a truncated series expansion of the first 2k + 2 terms, i.e.

$$u_{2k} = \sum_{n=0}^{2k+1} c_n(t)\varphi_n(x).$$
(3.12)

Let D and E denote (k + 1)-dimensional column vectors

$$D = [d_0, d_1, d_2, \cdots, d_k]^T$$
(3.13)

and

$$E = [e_0, e_1, e_2, \cdots, e_k]^T.$$
 (3.14)

Then the ODE systems (3.13) and (3.14) become

$$\frac{dD}{dt} = A_0 D \tag{3.15}$$

and

$$\frac{dE}{dt} = A_1 E \tag{3.16}$$

subject to some initial conditions, where

$$A_{0} = \begin{bmatrix} 0 & \sqrt{2} & 0 & 0 & \cdots \\ 0 & -2 & \sqrt{12} & 0 & \cdots \\ 0 & 0 & -4 & \sqrt{30} & \cdots \\ 0 & 0 & 0 & -6 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{bmatrix}$$
(3.17)

and

$$A_{1} = \begin{bmatrix} -1 & \sqrt{6} & 0 & 0 & \cdots \\ 0 & -3 & \sqrt{20} & 0 & \cdots \\ 0 & 0 & -5 & \sqrt{42} & \cdots \\ 0 & 0 & 0 & -7 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{bmatrix}.$$
 (3.18)

Since all the eigenvalues of A_1 are negative, we know that

$$\lim_{t \to \infty} E(t) = 0. \tag{3.19}$$

For the behavior of D(t) for large t, we need to know more about the eigenvectors of A_0 . We consider the eigenvectors of a matrix in the general case. Assume

$$A = \begin{bmatrix} \alpha_1 & \beta_1 & 0 & 0 & \cdots \\ 0 & \alpha_2 & \beta_2 & 0 & \cdots \\ 0 & 0 & \alpha_3 & \beta_3 & \cdots \\ 0 & 0 & 0 & \alpha_4 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{bmatrix}$$
(3.20)

where $\alpha_i, i = 1, 2, \dots, n$ are distinct real numbers and $\beta_i, i = 1, 2, \dots, n-1$ are nonzero real numbers. Obviously, $\alpha_1, \alpha_2, \alpha_3, \dots$ are the eigenvalues of A. Now, we try to find the eigenvector of A corresponding to α_i , which is denoted by

$$\mathbf{x}^{(i)} = [x_1^{(i)}, x_2^{(i)}, \cdots x_i^{(i)}, x_{i+1}^{(i)}, \cdots x_1^{(n)}].$$
(3.21)

Each $\mathbf{x}^{(i)}$ should be a nonzero solution of the following system:

$$\tilde{A}\mathbf{x}^{(i)} = 0 \tag{3.22}$$

where

$$\tilde{A} = \begin{bmatrix} \tilde{\alpha}_{1} & \beta_{1} & 0 & 0 & \cdots \\ 0 & \tilde{\alpha}_{2} & \beta_{2} & 0 & \cdots \\ 0 & 0 & \tilde{\alpha}_{3} & \beta_{3} & \cdots \\ 0 & 0 & 0 & \tilde{\alpha}_{4} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{bmatrix}$$
(3.23)

in which, $\tilde{\alpha}^{(k)} = \alpha^{(k)} - \alpha^{(i)} \neq 0$ since all the α 's are distinct. It is easily found that

$$x_k^{(i)} = 0, k = n, n - 1, \cdots, i + 1$$
 (3.24)

and

$$x_k^{(i)} = -\frac{\beta_k}{\tilde{\alpha}_k} x_{k+1}^{(i)}, k = i - 1, i - 2, \cdots, 1.$$
(3.25)

Therefore, $x_i^{(i)} \neq 0$, so we may choose $x_i^{(i)} = 1$. If we denote

$$X = [\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \cdots, \mathbf{x}^{(n)}],$$
(3.26)

where X is an upper triangular matrix with unitary diagonal entries, then

$$A = X\Lambda X^{-1}, \tag{3.27}$$

for

$$\Lambda = \operatorname{diag}[\alpha_1, \alpha_2, \cdots, \alpha_n]. \tag{3.28}$$

Thus for A_0 , we know that there is an upper triangular matrix with unitary diagonal entries T_0 such that

$$A_0 = T_0 \Lambda T_0^{-1}, \tag{3.29}$$

where

$$\Lambda = \text{diag}[0, -2, -4, \cdots, -2k]. \tag{3.30}$$

So, the solution D(t) could be expressed as :

$$D(t) = e^{A_0 t} d_0$$

= $T_0 e^{\Lambda t} T_0^{-1} d_0$ (3.31)

where d_0 is a (k+1)-dimensional vector and

$$e^{\Lambda t} = \text{diag}[1, e^{-2t}, e^{-4t}, \cdots e^{-2kt}].$$
 (3.32)

Therefore

$$\lim_{t \to \infty} D(t) = T_0 \operatorname{diag}[1, 0, \cdots, 0] T_0^{-1} \mathbf{d}_0$$

= $\operatorname{diag}(1, 0, \cdots, 0) T_0^{-1} \mathbf{d}_0$
= $[\overline{d}_0, 0, \cdots, 0]^T$, (3.33)

i.e., the behavior of the solution for the spectral method at large t is similar to φ_0 modular a constant multiplier, which coincides with the result for the static solution of the Fokker-Planck equation.

3.2 More general cases

Consider the following more general Fokker-Planck equation

$$\frac{\partial u}{\partial t} = \mu \frac{\partial (xu)}{\partial x} + \frac{\partial^2 u}{\partial x^2}$$
(3.34)

subject to initial condition:

$$u(0) = u_0 (3.35)$$

where μ is a constant.

By the relations (3.3) - (3.6) we could similarly get

$$c'_{n} = (1-\mu)\frac{(n(n-1))^{1/2}}{2}c_{n-2} + (\frac{1-\mu}{2}-n)c_{n} + (1+\mu)\frac{((n+1)(n+2))^{1/2}}{2}c_{n+2}$$
(3.36)
for $n = 0, 1, 2, \cdots,$

or,

$$d'_{k} = (1-\mu)\frac{(2k(2k-1))^{1/2}}{2}d_{k-1} + (\frac{1-\mu}{2}-2k)d_{k} + (1+\mu)\frac{((2k+1)(2k+2))^{1/2}}{2}d_{k+1}$$
(3.37)

and

$$e'_{k} = (1-\mu)\frac{(2k(2k+1))^{1/2}}{2}e_{k-1} + (\frac{1-\mu}{2} - 2k - 1)e_{k} + (1+\mu)\frac{((2k+2)(2k+3))^{1/2}}{2}e_{k+1}$$
(3.38)

for $k = 0, 1, 2, \cdots$ and where $d_k = c_{2k}, e_k = c_{2k+1}, k = 0, 1, 2, \cdots$. Taking an approximation of u as

$$u_{2k} = \sum_{n=0}^{2k+1} c_n(t)\varphi_n(x)$$
(3.39)

we get the following ODE systems for the approximate solution of the Fokker-Planck equation:

$$\frac{dD}{dt} = A_0 D \tag{3.40}$$

and

$$\frac{dE}{dt} = A_1 E, \tag{3.41}$$

where D, E are defined by (3.13), (3.14) with

$$A_{0} = \begin{bmatrix} \alpha_{0} & \gamma_{0} & & & \\ \beta_{0} & \alpha_{1} & \gamma_{1} & & \\ & \beta_{1} & \alpha_{2} & \ddots & \\ & & \ddots & \ddots & \gamma_{k-1} \\ & & & \beta_{k-1} & \alpha_{k} \end{bmatrix}$$
(3.42)

and

$$A_{1} = \begin{bmatrix} a_{0} & c_{0} & & & \\ b_{0} & a_{1} & c_{1} & & \\ & b_{1} & a_{2} & \ddots & \\ & & \ddots & \ddots & c_{k-1} \\ & & & b_{k-1} & a_{k} \end{bmatrix}$$
(3.43)

in which

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$$\alpha_i = \frac{\mu - 1}{2} - 2i \tag{3.44}$$

$$\beta_i = (1-\mu) \frac{((2k+1)(2k+2))^{1/2}}{2}$$
(3.45)

$$\gamma_i = (1+\mu) \frac{((2k+1)(2k+2))^{1/2}}{2}$$
 (3.46)

$$a_i = \frac{\mu - 1}{2} - 2i - 1 \tag{3.47}$$

$$b_i = (1-\mu) \frac{((2k+2)(2k+3))^{1/2}}{2}$$
(3.48)

$$c_i = (1+\mu) \frac{((2k+2)(2k+3))^{1/2}}{2}$$
(3.49)

for $i = 0, 1, 2 \cdots$.

Remark 3.1 If $1 < \mu < 3$ then $b_i c_i < 0$, $a_i < 0$. By the result given in Chapter 5, we know that all the eigenvalues of A_1 have negative real part, therefore the solution E(t) will approach 0 as t approaches to infinity. But for A_0 or for the other values of μ , it is not so clear theoretically.

3.3 Numerical Examples

In this section we give some numerical examples. In all these examples, the approximate solutions are taken as the sum of the first 2N + 2 terms in the expansion series of the solution.

Example 1. (The time-independent solution.) In chapter 2 we know that the static solution of the 1-D Fokker-Planck equation is

$$u_s = c\varphi_0, \tag{3.50}$$

where φ_0 is defined by (2.27). So, if the initial value $u_0 = \varphi_0$, then the solution obviously is $u(t) \equiv \varphi_0$. Figure 3.1 indicates the numerical result obtained by using our spectral method for this example. The numerical solution coincides with the static



Figure 3.1: The numerical solution with initial value $u_0 = \varphi_0$ solution since the solution is independent of t.

Figure 3.2: The numerical solution with initial value $u_0 = \varphi_2$

Example 2. (The time-dependent solution and its long-time behavior). We know that (3.50) is the static solution of the Fokker-Planck equation in which c is a constant determined by the integral of initial value u_0 , since

$$\int_{-\infty}^{+\infty} u(t)dx = \int_{-\infty}^{+\infty} u_0 dx.$$
(3.51)

So if we take $u_0 = \varphi_2$, we have

$$\int_{-\infty}^{+\infty} u_s dx = \lim_{t \to \infty} \int_{-\infty}^{+\infty} u(t) dx$$
$$= \int_{-\infty}^{+\infty} u_0 dx$$
$$= \int_{-\infty}^{+\infty} \varphi_2 dx$$
$$= \pi^{1/4}. \tag{3.52}$$

Combining the last equation and the fact that

$$\int_{-\infty}^{+\infty} \varphi_0 dx = \sqrt{2}\pi^{1/4},$$
 (3.53)

Figure 3.3: The numerical solution with $u_0 = \varphi_2$ at t = 0.5

we obtain

$$c = 1/\sqrt{2}.$$
 (3.54)

Figure 3.2 to Figure 3.6 illustrate the numerical results of our spectral method. It can be observed from these figures that as t is large the numerical solution approaches the static solution.

Example 3. If we take $u_0 = \varphi_8$, we can obtain

$$c = \frac{1}{8}\sqrt{\frac{35}{2}},\tag{3.55}$$

where c is the constant in the static solution defined by (3.50). Figure 3.7 and Figure 3.8 are the numerical solutions at small and large time, respectively.

Figure 3.4: The numerical solution with $u_0 = \varphi_2$ at t = 0.85

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Figure 3.5: The numerical solution with $u_0 = \varphi_2$ at t = 1.5

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Figure 3.7: The numerical solution with $u_0 = \varphi_8$ at t = 0.05

Figure 3.8: The numerical solution with $u_0 = \varphi_8$ at t = 3.0

Chapter 4

Spectral Method in two dimensional case

Now we turn to the following two-dimensional Fokker-Planck equation

$$\frac{\partial P}{\partial t} = -v\frac{\partial P}{\partial x} + \beta P + \left[\beta v + \frac{dU(x)}{dx}\right]\frac{\partial P}{\partial v} + \frac{\beta KT}{m\omega^2}\frac{\partial^2 P}{\partial v^2}$$
(4.1)

subject to initial data. Here U(x) is a given function defined by:

$$U(x) = \begin{cases} \frac{1}{2}(x+2)^2, & \text{if } x < -1\\ 1 - \frac{1}{2}x^2, & \text{if } -1 \le x \le 1\\ \frac{1}{2}(x-2)^2, & \text{if } x > 1 \end{cases}$$

To solve this equation, a number of numerical methods have been developed. In Cartling [7], difference method has been applied, whereas in Moore and Flaherty [17], Galerkin's method with adaptive mesh refinement techniques has been applied to the above Fokker-Planck equation. Numerical results are presented in both papers. In this chapter, we try to solve the Fokker-Planck equation by spectral method developed for the kinetic equation in Tang et al. [26]. All the techniques used in [26] work for the Fokker-Planck equation as well, but with some adaptations.

4.1 Series Expansion

Since the range of the variable v is $(-\infty, +\infty)$, it is natural to represent the unknown function P(x, v, t) by an expansion of Hermite polynomials in v with coefficients depending on x and t, i.e.,

$$P(x,v,t) = \sum_{n=0}^{\infty} d_n f_n(x,t) H_n(\alpha v) \exp(-\alpha^2 v^2), \qquad (4.2)$$

where $f_n(x,t), n = 1, 2, \cdots$ are unknown functions, α is a constant and H_n is the *n*-th order Hermite polynomial. We choose the factor $d_n = 1/\sqrt{2^n n!}$ so that the coefficient matrix of the induced partial differential equation system for f_n is symmetric, which implies this partial differential equation system is hyperbolic. We will see this later. For the sake of simplicity, we set

$$\ddot{H}(v) = d_n H_n(\alpha v) \exp(-\alpha^2 v^2).$$
(4.3)

Thus we could easily find the following recurrence relations among those functions:

$$\frac{d\tilde{H}_n(v)}{dv} = -\alpha \sqrt{2(n+1)}\tilde{H}_{n+1}(v), \qquad (4.4)$$

$$\frac{d^2 H_n(v)}{d^2 v} = \alpha^2 \sqrt{4(n+1)(n+2)} \tilde{H}_{n+2}(v), \qquad (4.5)$$

$$v\tilde{H}_{n}(v) = \frac{1}{\alpha} \left[\sqrt{\frac{n+1}{2}} \tilde{H}_{n+1}(v) + \sqrt{\frac{n}{2}} \tilde{H}_{n-1}(v) \right]$$
(4.6)

and

$$v\frac{d\tilde{H}_n(v)}{dv} = -\sqrt{(n+1)(n+2)}\tilde{H}_{n+2}(v) - (n+1)\tilde{H}_n(v).$$
(4.7)

From these relations, we have

$$-v\frac{\partial P}{\partial x}$$

= $-\sum_{n=0}^{\infty} \frac{1}{\alpha} \left[\sqrt{\frac{n+1}{2}} \tilde{H}_{n+1}(v) + \sqrt{\frac{n}{2}} \tilde{H}_{n-1}(v) \right] \frac{\partial f_n}{\partial x}$

$$= -\frac{1}{\alpha} \sum_{n=0}^{\infty} \sqrt{\frac{n+1}{2}} \tilde{H}_{n+1}(v) \frac{\partial f_n}{\partial x} - \frac{1}{\alpha} \sum_{n=0}^{\infty} \sqrt{\frac{n}{2}} \tilde{H}_{n-1}(v) \frac{\partial f_n}{\partial x}$$
$$= -\frac{1}{\alpha} \sum_{n=0}^{\infty} \left[\sqrt{\frac{n}{2}} \frac{\partial f_{n-1}}{\partial x} + \sqrt{\frac{n+1}{2}} \frac{\partial f_{n+1}}{\partial x} \right] \tilde{H}_n(v).$$
(4.8)

Similarly, we can obtain

$$\frac{\partial(vP)}{\partial v} = -\sum_{n=0}^{\infty} (\sqrt{(n-1)n} f_{n-2} + n f_n) \tilde{H}_n(v), \qquad (4.9)$$

$$\frac{\partial P}{\partial v} = \alpha \sum_{n=0}^{\infty} \sqrt{2n} f_{n-1} \tilde{H}_n(v)$$
(4.10)

and

$$\frac{\partial^2 P}{\partial v^2} = \alpha^2 \sum_{n=0}^{\infty} 2\sqrt{(n+1)n} f_{n-2} \tilde{H}_n(v), \qquad (4.11)$$

where $f_{-1} = f_{-2} = 0$. Substituting all these into equation (4.1) and equating the coefficient of $\tilde{H}_n(v)$ on the two sides of the equation, we obtain the following partial differential equation system:

$$\frac{\partial f_n}{\partial t} = -\frac{1}{\alpha} \left[\sqrt{\frac{n}{2}} \frac{\partial f_{n-1}}{\partial x} + \sqrt{\frac{n+1}{2}} \frac{\partial f_{n+1}}{\partial x} \right] - n\beta f_n \\ -\sqrt{2}\alpha \frac{dU(x)}{x} \sqrt{n} f_{n-1} + (2\alpha^2 \mu - \beta) \sqrt{(n-1)n} f_{n-2}, \qquad (4.12)$$

$$\frac{\partial f_n}{\partial t} = -\frac{1}{\alpha} \left[\sqrt{\frac{n}{2}} \frac{\partial f_{n-1}}{\partial x} + \sqrt{\frac{n+1}{2}} \frac{\partial f_{n+1}}{\partial x} \right] \\ + d_{n0} f_n + d_{n(-1)} f_{n-1} + d_{n(-2)} f_{n-2}$$
(4.13)

where

$$d_{n0} = -\beta n, \qquad (4.14)$$

$$d_{n(-1)} = -\sqrt{2\alpha} \frac{dU(x)}{dx} \sqrt{n}, \qquad (4.15)$$

$$d_{n(-2)} = \beta(2\alpha^2\mu - 1)\sqrt{(n-1)n}$$
 (4.16)

or,

and

$$\mu = KT/m\omega^2, \qquad (4.17)$$

for $n = 0, 1, 2, \cdots$.

4.2 Spectral Method

The spectral method of order N consists of solving the first N + 1 equations of (4.13) for the N + 1 unknown functions $f_0, f_1, f_2, \dots f_N$. All the functions $f_n, n \ge N + 1$, are set to 0, i.e. take the approximate solution to P(x, v, t) as the following truncated series $P_N(x, v, t)$

$$P_N(x,v,t) = \sum_{n=0}^N \frac{1}{\sqrt{2^n n!}} f_n(x,t) H_n(\alpha v) \exp(-\alpha^2 v^2).$$
(4.18)

Let f denote a (N + 1)-dimensional column vector defined by

$$\mathbf{f} = \mathbf{f}(x,t) = [f_0(x,t), f_1(x,t), \cdots, f_N(x,t)]^T.$$
(4.19)

Then equations (4.13) become

$$\frac{\partial \mathbf{f}}{\partial t} = -\frac{1}{\alpha} R \frac{\partial \mathbf{f}}{\partial x} + S \mathbf{f}$$
(4.20)

where R and S are $(N+1) \times (N+1)$ matrices given by

$$R = \begin{bmatrix} 0 & \alpha_{1} & & & \\ \alpha_{1} & 0 & \alpha_{2} & & \\ & \alpha_{2} & 0 & \ddots & \\ & & \ddots & \ddots & \alpha_{N} \\ & & & \alpha_{N} & 0 \end{bmatrix}$$
(4.21)

and

$$S = \begin{bmatrix} d_{00} & & & \\ d_{1(-1)} & d_{10} & & & \\ d_{2(-2)} & d_{2(-1)} & d_{20} & & \\ & & & \\ & & & \\ & & & \\ 0 & & \ddots & \ddots & \\ & & & & \\ & & & & \\ & & & & \\ & & & \\ &$$

in which $\alpha_n = \sqrt{n/2}, n = 1, 2, \dots, N$ and $d_{n0}, d_{n(-1)}, d_{n(-2)}, n = 0, 1, \dots, N$ are defined by (4.14)-(4.16), plus initial data.

Obviously, R is a symmetric matrix, and thus has N + 1 real eigenvalues. Furthermore, we have

Theorem 4.1 (See [26]) The eigenvalues of R are the zeroes of the (N+1)-th order Hermite polynomial $H_{N+1}(\lambda)$.

Proof. Let $p_{N+1}(\lambda)$ be the characteristic polynomial of R. Since R is tridiagonal, we have

$$p_{N+1} = \lambda p_N(\lambda) - \alpha_N^2 p_{N-1}(\lambda)$$

= $\lambda p_N(\lambda) - \frac{N}{2} p_{N-1}(\lambda)$ (4.23)

for $N = 2, 3, 4, \cdots$ and

$$p_1 = \lambda, \qquad (4.24)$$

$$p_2 = \lambda^2 - \frac{1}{2}.$$
 (4.25)

We shall prove that

$$p_N = 2^{-N} H_N \text{ for } n \ge 1$$
 . (4.26)

Obviously this is true for N = 1, 2. Assume (4.26) is true for $N \le n$. From (4.23) and the recurrence relations among Hermite polynomials, we have

$$p_{n+1} = \lambda p_n(\lambda) - \frac{n}{2} p_{n-1}(\lambda)$$

$$= \lambda 2^{-n} H_n(\lambda) - n 2^{-n} H_{n-1}(\lambda)$$

= $2^{-(n+1)} (2\lambda H_n(\lambda) - 2n H_{n-1}(\lambda)).$ (4.27)

This completes the proof of the theorem. \Box

Let $\lambda_0 < \lambda_1 < \cdots < \lambda_N$ be the zeros of the Hermite polynomial H_{N+1} and C_k be defined by

$$C_k = \{\sum_{n=0}^{N} \frac{1}{2^n n!} [H_n(\lambda_k)]^2\}^{-1/2}.$$
(4.28)

We have the following result regarding the eigenvectors of R.

Theorem 4.2 (See [26]) The eigenvector of R corresponding to the eigenvalue λ_k can be given by

$$\mathbf{u}_k = [u_{0k}, u_{1k}, \cdots, u_{Nk}]^T$$
 (4.29)

in which u_{nk} is defined by

$$u_{nk} = \frac{C_k}{\sqrt{2^n n!}} H_n(\lambda_k). \tag{4.30}$$

Proof. Assume that an eigenvector of R corresponding to λ_k is

$$\mathbf{y} = [y_0, y_1, \cdots, y_N]^T.$$
 (4.31)

Then

$$R\mathbf{y} = \lambda_k \mathbf{y}.\tag{4.32}$$

This is equivalent to the following difference equation

$$\sqrt{\frac{n}{2}}y_{n-1} + \sqrt{\frac{n+1}{2}}y_{n+1} = \lambda_k y_n, \quad n = 0, 1, \cdots, N$$
(4.33)

with boundary conditions $y_{-1} = y_{N+1} = 0$. This could be directly verified by setting $y_n = u_{nk}$ noticing the fact that $H_{N+1}(\lambda_k) = 0$. The theorem is therefore proved. \Box

Obviously the eigenvectors defined by (4.29) are normalized and they are mutually orthogonal since R is a symmetric matrix. Let matrix U be defined by

$$U = [\mathbf{u}_0, \mathbf{u}_1, \cdots, \mathbf{u}_N]. \tag{4.34}$$

then U is an orthogonal matrix and

$$U^{T}RU = \Lambda = \operatorname{diag}[\lambda_{0}, \lambda_{1}, \cdots, \lambda_{N}].$$
(4.35)

If we premultiply (4.20) by U^T , we obtain

$$\frac{\partial \tilde{\mathbf{f}}}{\partial t} = -\frac{1}{\alpha} \Lambda \frac{\partial \tilde{\mathbf{f}}}{\partial x} + \tilde{S} \tilde{\mathbf{f}}$$
(4.36)

by letting $\tilde{\mathbf{f}} = U^T \mathbf{f}$ and $\tilde{S} = U^T S U$.

Eq. (4.36) is a typical hyperbolic system. Since the entries of the diagonal matrix Λ change signs, we need to consider different finite difference approximations for $\lambda_i \frac{\partial \tilde{f}_i}{\partial x}$ according to the signs of $\lambda_i, 0 \leq i \leq N$ in order to ensure the stability of the difference methods. If $\lambda_i > 0$, the backward space difference scheme

$$\lambda_i \frac{\partial \tilde{f}_i}{\partial x} \approx \frac{\lambda_i}{\Delta y} (\tilde{f}_i(x,t) - \tilde{f}_i(x - \Delta x, t))$$
(4.37)

should be used. If $\lambda_i < 0$, the forward space difference scheme

$$\lambda_i \frac{\partial \tilde{f}_i}{\partial x} \approx \frac{\lambda_i}{\Delta y} (\tilde{f}_i(x + \Delta x, t) - \tilde{f}_i(x, t))$$
(4.38)

should be used. Therefore, the numerical scheme for (4.36) is

$$\tilde{f}_{i}(x,t+\Delta t) = \tilde{f}_{i}(x,t) - \frac{\lambda_{i}}{\alpha} \frac{\Delta t}{\Delta y} (\tilde{f}_{i}(x,t) - \tilde{f}_{i}(x-\Delta x,t))
+ \Delta t (\tilde{S}\tilde{\mathbf{f}})_{i}(x,t), \quad \text{if } \lambda_{i} > 0;$$
(4.39)

$$\tilde{f}_{i}(x,t+\Delta t) = \tilde{f}_{i}(x,t) - \frac{\lambda_{i}}{\alpha} \frac{\Delta t}{\Delta y} (\tilde{f}_{i}(x+\Delta x,t) - \tilde{f}_{i}(x,t))
+ \Delta t (\tilde{S}\tilde{\mathbf{f}})_{i}(x,t), \quad \text{if } \lambda_{i} < 0;$$
(4.40)

$$\tilde{f}_i(x,t+\Delta t) = \tilde{f}_i(x,t) + \Delta t(\tilde{S}\tilde{f})_i(x,t), \quad \text{if } \lambda_i = 0.$$
(4.41)

It is easy to see that the above scheme (4.39)-(4.41) can produce stable solutions for the hyperbolic system (4.36).

Originally, system (4.20) is a Cauchy problem and we know that only those solutions which go to zero as t goes to infinity make sense in physics. So we may turn the

Cauchy problem into an initial-boundary problem by setting the following artificial boundary conditions:

$$\tilde{f}_j(M,t) = 0 \quad \forall t \ge 0, j = 0, 1, 2, \cdots, \frac{N-1}{2}$$
 (4.42)

 $\quad \text{and} \quad$

$$\tilde{f}_j(-M,t) = 0 \quad \forall t \ge 0, j = \frac{N+1}{2}, \frac{N+1}{2} + 1, \cdots, N$$
 (4.43)

when N is odd; and

$$\tilde{f}_j(M,t) = 0 \quad \forall t \ge 0, j = 0, 1, \cdots, \frac{N}{2} - 1$$
 (4.44)

and

$$\tilde{f}_j(-M,t) = 0 \quad \forall t \ge 0, j = \frac{N}{2} + 1, \frac{N}{2} + 2, \cdots, N$$
 (4.45)

when N is even.

Chapter 5

The eigenvalues of tridiagonal matrices

Tridiagonal matrices are very common and important in many applications. For the eigenvalue problem of symmetric tridiagonal matrices, extensive theoretical and numerical work can be found in the literature. In this chapter, we will investigate the eigenvalue distribution of some class of non-symmetric tridiagonal matrices. This class of matrices would arise from the spectral method for the Fokker-Planck equation when Hermite polynomials are employed. We have seen this in chapter 3 and we will see the details in the following section.

Denote a $n \times n$ tridiagonal matrix by A_n :

$$A_{n} = \begin{bmatrix} \alpha_{1} & \beta_{1} & & & \\ \gamma_{1} & \alpha_{2} & \beta_{2} & & \\ & \gamma_{2} & \alpha_{3} & \ddots & \\ & & \ddots & \ddots & \beta_{n-1} \\ & & & \gamma_{n-1} & \alpha_{n} \end{bmatrix}$$
(5.1)

where $\beta_j \gamma_j < 0, j = 1, 2, \dots, n-1$. Under this condition we may prove that A_n is

similar to a matrix

$$\tilde{A}_{n} = \begin{bmatrix} \alpha_{1} & \tilde{\beta}_{1} & & \\ -\tilde{\beta}_{1} & \alpha_{2} & \tilde{\beta}_{2} & & \\ & -\tilde{\beta}_{2} & \alpha_{3} & \ddots & \\ & & \ddots & \ddots & \tilde{\beta}_{n-1} \\ & & & -\tilde{\beta}_{n-1} & \alpha_{n} \end{bmatrix}$$
(5.2)

where all $\tilde{\beta}_j, j = 1, 2, \dots, n-1$ are positive. In fact, by taking $D = \text{diag}[d_1, d_2, d_3, \dots, d_n], d_j \neq 0, j = 1, 2, \dots, n$, we have

$$DA_{n}D^{-1} = \begin{bmatrix} \alpha_{1} & b_{1} & & \\ c_{1} & \alpha_{2} & b_{2} & & \\ & c_{2} & \alpha_{3} & \ddots & \\ & & \ddots & \ddots & b_{n-1} \\ & & & c_{n-1} & \alpha_{n} \end{bmatrix}$$
(5.3)

where

$$b_j = d_j \beta_j d_{j+1}^{-1} c_j = d_{j+1} \gamma_j d_j^{-1}$$
(5.4)

for $j = 1, 2, 3, \dots, n$. Thus we may choose some d_j for each $j = 1, 2, 3, \dots, n$, such that

$$b_j = c_j > 0, j = 1, 2, 3, \cdots, n,$$
 (5.5)

i.e.,

$$d_{j+1}^2 = -\frac{\gamma_j}{\beta_j} d_j^2, j = 1, 2, 3, \cdots, n.$$
 (5.6)

Therefore we may assume $\gamma_j = -\beta_j < 0, j = 1, 2, 3, \dots, n$ in (5.1) without loss of generality. We still denote this matrix by A_n , i.e.

$$A_{n} = \begin{bmatrix} \alpha_{1} & \beta_{1} & & \\ -\beta_{1} & \alpha_{2} & \beta_{2} & & \\ & -\beta_{2} & \alpha_{3} & \ddots & \\ & & \ddots & \ddots & \beta_{n-1} \\ & & & -\beta_{n-1} & \alpha_{n} \end{bmatrix}.$$
 (5.7)

Then we have the following theorem for such types of matrices:

Theorem 5.1 If all the diagonal entries in A_n are strictly positive, all the eigenvalues of A_n are on the right half complex plane.

Before we prove this theorem, we need to prove some auxiliary results. Let $B(t), D, C_n$ be respectively defined as follows:

$$B_{n}(t) = \begin{bmatrix} -t & \beta_{1} & & & \\ \beta_{1} & -t & \beta_{2} & & \\ & \beta_{2} & -t & \ddots & \\ & & \ddots & \ddots & \beta_{n-1} \\ & & & & \beta_{n-1} & -t \end{bmatrix},$$
(5.8)

$$D = \operatorname{diag}[\alpha_1, \alpha_2, \alpha_3, \cdots, \alpha_n]$$
(5.9)

and

$$C_{n} = \begin{bmatrix} i\alpha_{1} & \beta_{1} & & & \\ \beta_{1} & i\alpha_{2} & \beta_{2} & & \\ & \beta_{2} & i\alpha_{3} & \ddots & \\ & & \ddots & \ddots & \beta_{n-1} \\ & & & & \beta_{n-1} & i\alpha_{n} \end{bmatrix}$$
(5.10)

where i is the imaginary unit. Using the matrices defined above we have

Theorem 5.2 iA_n and C_n have the same characteristic polynomials, therefore they have the same set of eigenvalues.

Proof. Both iA_n and C_n are tridiagonal matrices, thus we know that the recurrence relations for them are

$$det(iA_n - zI) = (i\alpha_n - z)det(iA_{n-1} - zI) + (i\beta_{n-1})^2 det(iA_{n-2} - zI)$$

= $(i\alpha_n - z)det(iA_{n-1} - zI) - \beta_{n-1}^2 det(iA_{n-2} - zI)$ (5.11)

and

$$\det(C_n - zI) = (i\alpha_n - z)\det(C_{n-1} - zI) - \beta_{n-1}^2\det(C_{n-2} - zI)$$
 (5.12)

for $n = 3, 4, 5, \cdots$. It can be easily verified that

$$\det(iA_n - zI) \equiv \det(C_n - zI) \tag{5.13}$$

for n = 1, 2. Therefore both characteristic polynomials are identical for any integer number n. \Box

Theorem 5.3 C_n has no real eigenvalue if all $\alpha_i, i = 1, 2, \dots, n$ are strictly positive. **Proof.** Assume that C_n has a real eigenvalue t and let $\mathbf{x} + i\mathbf{y}$ be the corresponding eigenvector. Then we have

$$C_n(\mathbf{x} + i\mathbf{y}) = t(\mathbf{x} + i\mathbf{y}), \tag{5.14}$$

or,

$$(B(t) + iD)(\mathbf{x} + i\mathbf{y}) = \mathbf{0}.$$
 (5.15)

(5.15) can be rewritten as

$$B(t)\mathbf{x} - D\mathbf{y} = \mathbf{0} \tag{5.16}$$

and

$$B(t)\mathbf{y} + D\mathbf{x} = \mathbf{0} \tag{5.17}$$

or,

$$\begin{bmatrix} B(t) & -D \\ D & B(t) \end{bmatrix} \begin{bmatrix} \mathbf{x} \\ \mathbf{y} \end{bmatrix} = \mathbf{0}.$$
 (5.18)

But

$$\begin{bmatrix} 0 & I \\ I & -B(t)D^{-1} \end{bmatrix} \begin{bmatrix} B(t) & -D \\ D & B(t) \end{bmatrix} = \begin{bmatrix} D & B(t) \\ 0 & -(B(t)D^{-1}B(t) + D) \end{bmatrix}$$
(5.19)

thus

$$\det \begin{bmatrix} B(t) & -D \\ D & B(t) \end{bmatrix} = \pm \det(D)\det(B(t)D^{-1}B(t) + D).$$
 (5.20)

On the other hand,

$$(B(t)D^{-1}B(t) + D) = D^{\frac{1}{2}}((D^{-\frac{1}{2}}B(t)D^{-\frac{1}{2}})^2 + I)D^{\frac{1}{2}}$$
(5.21)

and $D^{-\frac{1}{2}}B(t)D^{-\frac{1}{2}}$ is a symmetric matrix so that $B(t)D^{-1}B(t)+D$ is a positive definite matrix. Therefore, system (5.18) has only the trivial solution. This is contradictory to the assumption at the beginning. \Box

Theorem 5.4 A_n has no pure imaginary eigenvalue under the same condition in Theorem 5.1.

Proof. This is quite staightforward since iA_n and C_n have the same set of eigenvalues. \Box

Now a proof of Theorem 5.1 could be given. **Proof** of Theorem 5.1. Let

$$A_n(s) = \begin{bmatrix} \alpha_1 & s\beta_1 & & \\ -s\beta_1 & \alpha_2 & s\beta_2 & & \\ & -s\beta_2 & \alpha_3 & \ddots & \\ & & \ddots & \ddots & s\beta_{n-1} \\ & & & -s\beta_{n-1} & \alpha_n \end{bmatrix}.$$
 (5.22)

Then $A(0) = D, A(1) = A_n$ and all the eigenvalues of $A(s), \lambda_j, j = 1, 2, \dots, n$, are continuous functions of s since eigenvalues of a matrix are continuous functions of its entries. When s = 0, obviously $\lambda_j(0) = \alpha_j, j = 1, 2, \dots, n$; thus all eigenvalues are on the right half plane. For any $0 < s \leq 1$, the condition in Theorem 5.1 for A_n is satisfied, thus A(s) has no pure imaginary eigenvalue. Therefore, no eigenvalue of A(s) can go to the left half plane without crossing the imaginary axis. This implies that all the eigenvalues of A(s) stay on the right half plane, i.e.,

$$Re\{\lambda_j(s)\} > 0, j = 1, 2, \cdots, n.$$
 (5.23)

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In particular,

$$Re\{\lambda_j\} = Re\{\lambda_j(1)\} > 0, j = 1, 2, \cdots, n$$
(5.24)

where $\lambda_j, j = 1, 2, \dots, n$ are the eigenvalues of A_n .

As a consequence of Theorem 5.1, we have:

Theorem 5.5 If all diagonal entries in A_n are strictly negative, then all eigenvalues of A_n are on the left half plane.

Furthermore we have the following result under a slightly different condition.

Theorem 5.6 If A_n satisfies the conditions in Theorem 5.1 except that $\alpha_1 = 0$, the statement in Theorem 5.1 is still true.

Proof. From the proof of Theorem 5.1 we know that the key point is to show that the matrix in system (5.18) is nonsingular, or to show that the following matrix

$$T = \begin{bmatrix} D & B(t) \\ B(t) & -D \end{bmatrix}$$
(5.25)

is nonsingular for any real number t. Let

$$D = \begin{bmatrix} 0 & 0^T \\ 0 & D_1 \end{bmatrix}$$
(5.26)

and

$$B(t) = \begin{bmatrix} -t & \mathbf{b}_1^T \\ \mathbf{b}_1 & B_1(t) \end{bmatrix}.$$
 (5.27)

Then D_1 is positive definite. There can be only two cases for t:

(i) t is not eigenvalue of B(0) then B(t) is invertible;

:: .

(ii) t is an eigenvalue of B(0), then t is not an eigenvalue of $B_1(0)$ and thus $B_1(t)$ is invertible.

Case (i). We have

$$\begin{bmatrix} I & 0 \\ -DB^{-1}(t) & I \end{bmatrix} \begin{bmatrix} B(t) & -D \\ D & B(t) \end{bmatrix} = \begin{bmatrix} B(t) & -D \\ D & DB^{-1}(t)D + B(t) \end{bmatrix}$$
(5.28)

so,

$$\det \begin{bmatrix} B(t) & -D \\ D & B(t) \end{bmatrix} = \pm \det(B(t))\det(DB^{-1}(t)D + B).$$
 (5.29)

Similar to the proof of Theorem 5.1 it could be verified that above determinant is nonzero.

Case (ii). For simplicity we will drop t in $B_1(t)$ and denote both 0 and 0^T by 0 from now on. We can make following multiplication for T:

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & I & 0 & 0 \\ 0 & -\mathbf{b}_{1}^{T} D_{1}^{-1} & 1 & 0 \\ 0 & -B_{1} D_{1}^{-1} & 0 & I \end{bmatrix} \begin{bmatrix} 0 & 0 & -t & \mathbf{b}_{1}^{T} \\ 0 & D_{1} & \mathbf{b}_{1} & B_{1} \\ -t & \mathbf{b}_{1}^{T} & 0 & 0 \\ \mathbf{b}_{1} & B_{1} & 0 & D_{1} \end{bmatrix}$$
$$= \begin{bmatrix} 0 & 0 & -t & \mathbf{b}_{1}^{T} \\ 0 & D_{1} & \mathbf{b}_{1} & B_{1} \\ -t & 0 & -\mathbf{b}_{1}^{T} D_{1}^{-1} \mathbf{b}_{1} & -\mathbf{b}_{1}^{T} D_{1}^{-1} B_{1} \\ \mathbf{b}_{1} & 0 & -B_{1} D_{1}^{-1} \mathbf{b}_{1} & -(B_{1} D_{1}^{-1} B_{1} + D_{1}^{-1}) \end{bmatrix}$$
(5.30)

Let

$$\mathbf{b}_2 = B_1 D_1^{-1} \mathbf{b}_1, \tag{5.31}$$

$$c_1 = \mathbf{b}_1^T D_1^{-1} \mathbf{b}_1 \tag{5.32}$$

and

$$E = B_1 D_1^{-1} B_1 + D_1^{-1} (5.33)$$

Then it is not difficult to prove that E is positive definite since D_1 is positive definite and B_1 is symmetric. From this notation one sees that

$$\begin{bmatrix} 1 & 0 & \mathbf{b}_{1}^{T} E^{-1} \\ 0 & 1 & -\mathbf{b}_{2}^{T} E^{-1} \\ 0 & 0 & I \end{bmatrix} \begin{bmatrix} 0 & -t & \mathbf{b}_{1}^{T} \\ -t & -c_{1} & -\mathbf{b}_{2}^{T} \\ \mathbf{b}_{1} & -\mathbf{b}_{2} & -E \end{bmatrix}$$

$$= \begin{bmatrix} \mathbf{b}_{1}^{T} E^{-1} \mathbf{b}_{1} & -(t + \mathbf{b}_{1}^{T} E^{-1} \mathbf{b}_{2}) & 0 \\ -(t + \mathbf{b}_{2}^{T} E^{-1} \mathbf{b}_{1}) & \mathbf{b}_{2}^{T} E^{-1} \mathbf{b}_{2} - c_{1} & 0 \\ \mathbf{b}_{1} & -\mathbf{b}_{2} & -E \end{bmatrix}.$$
(5.34)

Therefore,

=

$$\det(T) = \pm \det(D_1)\det \begin{bmatrix} 0 & -t & \mathbf{b}_1^T \\ -t & -c_1 & -\mathbf{b}_2^T \\ \mathbf{b}_1 & -\mathbf{b}_2 & -E \end{bmatrix}$$

$$\pm \det(D_1\det(E)[\mathbf{b}_1^T E^{-1}\mathbf{b}_1(\mathbf{b}_2^T E^{-1}\mathbf{b}_2 - c_1) - (t + \mathbf{b}_1^T E^{-1}\mathbf{b}_2)^2]$$
(5.35)

since $\mathbf{b}_1^T E^{-1} \mathbf{b}_2 = \mathbf{b}_2^T E^{-1} \mathbf{b}_1$. Thus we only need to prove that

$$c_1 - \mathbf{b}_2^T E^{-1} \mathbf{b}_2 > 0, \tag{5.36}$$

or,

$$P = D_1^{-1} - D_1^{-1} B_1 E^{-1} B_1 D_1^{-1} > 0.$$
 (5.37)

From (5.33) we know that

$$E^{-1}(B_1D_1^{-1}B_1 + D_1^{-1}) = I.$$
 (5.38)

So,

$$P = D_{1}^{-1} - D_{1}^{-1} B_{1} (B_{1}^{-1} - E^{-1} D_{1} B_{1}^{-1})$$

$$= D_{1}^{-1} B_{1} E^{-1} D_{1} B_{1}^{-1}$$

$$= D_{1}^{-\frac{1}{2}} [(D_{1}^{-\frac{1}{2}} B_{1}) E^{-1} (D_{1}^{-\frac{1}{2}} B_{1})^{-1}] D_{1}^{-\frac{1}{2}}$$

$$= D_{1}^{-\frac{1}{2}} P_{1} D_{1}^{-\frac{1}{2}}$$
(5.39)

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	α's	β 's	eigenvalues
1	0	6	-0.0000 + 8.3666i
2	0	5	-0.0000 - 8.3666i
3	0	4	-0.0037 + 4.2802i
4	0	3	-0.0037 - 4.2802i
5	0	2	-0.1340 + 1.5688i
6	0	1	-0.1340 - 1.5688i
7	-1		-0.7247

Table 5.1: The statement not true for k = 6.

where $P_1 = (D_1^{-\frac{1}{2}}B_1)E^{-1}(D_1^{-\frac{1}{2}}B_1)^{-1}$. Therefore all eigenvalues of P_1 are strictly positive since E^{-1} is positive and similar to P_1 , and P is positive definite. \Box

Remark 5.1 An interesting question is, if $\alpha_i = 0, 1 \le i \le k < n$, does the result still hold? Some numerical examples indicate that k could be larger than one, but what is the largest k? This is attractive to me and maybe to some readers as well.

Examples. Table 5.1 to Table 5.4 give some examples of the eigenvalues of tridiagonal matrices. From Table 5.1 and Table 5.2, we see that the real part of the first two eigenvalues should be zero. The next two tables show the cases that k = 5, 6respectively.

	α's	β 's	eigenvalues
1	0	6	-0.0000 + 8.3665i
2	0	5	-0.0000 - 8.3665i
3	0	4	-0.0055 + 4.2675i
4	0	3	-0.0055 - 4.2675i
5	0	2	-0.0431 + 1.3503i
6	0	1	-0.0431 - 1.3503i
7	-10		-9.9027

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Table 5.2: The statement not true for k = 6 for another matrix.

	α 's	β 's	eigenvalues
1	0	6	-0.0007 + 8.3665i
2	0	5	-0.0007 - 8.3665i
3	0	4	-0.0704 + 4.2622i
4	0	3	-0.0704 - 4.2622i
5	0	2	-0.6032 + 1.5545i
6	-1	1	-0.6032 - 1.5545i
7	-1		-0.6515

Table 5.3: The statement true for k = 5

	α's	β 's	eigenvalues
1	0	1	-0.2123 + 8.3463i
2	0	2	-0.2123 - 8.3463i
3	0	3	-0.0660
4	0	4	-0.1026 + 1.6318i
5	0	5	-0.1026 - 1.6318i
6	0	6,	-0.1521 + 4.2729i
7	-1		-0.1521 - 4.2729i

Table 5.4: The statement true for k = 6.

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