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Analytic properties of the recursion method in the presence of band gaps†

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Abstract. The recursion method gives a good approximation of the density of states in the single-band case, where the recursion coefficients converge. When band gaps exist, it is known that they exhibit asymptotic undamped oscillations. In order to clarify these asymptotic behaviours, an analytic study of the recursion method applicable to the band-gap case is presented. The asymptotic properties of the system of orthogonal polynomials, to which this method is closely related, are investigated by use of the concept of the exterior mapping function. Various relations, which connect the means of the recursion coefficients to the support of a spectrum, are obtained. The period of their asymptotic oscillations is written as a function of the support. The numerical results by Turchi, Ducastelle and Tréglia can be well interpreted by the present theory. The asymptotic properties of the truncated basis are also examined.

1. Introduction

Since the recursion method was introduced by Haydock *et al* (1972), it has been successfully used to investigate the electronic structure or the vibrational spectrum of the system, where its Hamiltonian or its force matrix is written in the tight-binding form (for a review see Haydock (1980) and Kelly (1980)). This method gives an approximation of the diagonal element of the resolvent, which is expressed in the continued fraction form by use of the recursion coefficients. Here the recursion coefficients are computed successively from the Hamiltonian and the state on which the diagonal element is taken.

It has been empirically known that this method reproduces the density of states quite well in the single-band (no band gap) case, where the recursion coefficients seem to converge, and this convergence is essential for the facility of this method. On the contrary when the band gap exists (multiband case), it was soon pointed out that the recursion coefficients do not converge and exhibit undamped oscillations (Gaspard and Cyrot-Lackman 1973), which is a natural consequence since their convergence implies the single band. Therefore the recursion method has been scarcely used in the multiband case.

Although the convergence of the recursion coefficients in the single-band case had been confirmed numerically in many examples, the reason or the condition for the convergence was not necessarily fully understood. Several years later Magnus (1979)

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pointed out that in the single-band case the rigorous description of the recursion method is possible by using the Szegö theory (Szegö 1958) on the asymptotic forms of general orthogonal polynomials. The correspondence between the recursion method and the system of orthogonal polynomials with an adequate weight is easy to derive in the case where the spectral function is well defined. If the band is single and its spectral form satisfies a certain condition (Szegö condition), the empirical law of the convergence can be proved through this correspondence. Magnus also examined the multiband case, which is related to the orthogonal polynomials whose weight has a system of intervals as the support, but the obtained result seems to be less fruitful than in the single-band case (see also Magnus 1985). The orthogonal polynomials defined on a system of intervals have been far less investigated than those on a single interval (see, e.g., Ahiezer (1960) and Nuttall and Singh (1977)), and so in order to treat the multiband case, it is necessary to develop the theory on such orthogonal polynomials.

A few years ago Turchi *et al* (1982, here referred to as TDT) carried out extensive numerical experiments on the recursion coefficients, mainly in the two-band case, and revealed the characteristic features of their asymptotic behaviours. According to the TDT results (see also Haydock and Nex (1985)) their asymptotic oscillations seem to be incommensurate in general and to depend only on the positions of the band edges (including also the inner edges constituting the band gap), i.e. the support of the spectrum. If two sub-bands have the bandwidths of the same order (about less than a factor of two), then the sequences of the recursion coefficients look like a mixture of two oscillating subsequences with the same period. The diagonal element of the resolvent was also reconstructed by an adequate termination of the coefficients.

These results leave some problems unsolved. For example, one does not know what quantity determines the period of the asymptotic oscillations, although it seems to be written as a function of the support. If one computes the eigenvalues of the truncated Hamiltonian, then what information do these eigenvalues give? These problems may be solved by a similar theory in the multiband case as the Szegö theory in the single-band case.

In this paper an analytic description of the orthogonal polynomials associated with a system of intervals is given with the main interest in their asymptotic behaviours, and a clear insight into the asymptotic properties of the recursion method in the general multiband case will be gained. The limiting forms of the orthogonal polynomials are examined by use of a special field in analytic function theory, which is familiar in potential theory (Tsuji 1959) but is not necessarily familiar in the theory of condensed matter.

Our theory is outlined as follows. First we introduce the fundamental theorem which says that one can define a family of polynomials whose limit forms are written by the (generalised) exterior mapping function (EMF). Next the system of orthogonal polynomials is shown to belong to this family under a certain condition (the Geronimus condition) which can be regarded as being satisfied in the ordinary case, and as a consequence the asymptotic behaviours of the recursion coefficients are investigated in relation to the EMF. The EMF is closely related to the complex potential in two-dimensional electrostatics, and thus its explicit form can be written through the problem of the electrostatic potential.

This paper is organised as follows. First in § 2, the recursion method is formulated in the form convenient for the present theory, and its relationship to the system of orthogonal polynomials is described. Section 3 is devoted to the introduction to the EMF and the above-mentioned fundamental theorem. In § 4 the Geronimus condition and the explicit form of the EMF are given, and as a consequence a set of limit relations of the recursion coefficients is derived. The period of their asymptotic oscillations is also considered. A good agreement with the TDT numerical results is found. The asymptotic properties of the truncated basis are analysed in § 5, and some simple cases are treated in § 6. Finally in § 7 the results of this work are summarised.

2. Preliminaries

Our problem is described as follows: when the Hamiltonian H and an arbitrary normalised state, which we call $|0\rangle$, are given, then how do we approximate the diagonal element of the resolvent denoted by $G(z)=\langle 0|(z-H)^{-1}|0\rangle$? Here we consider the case where its spectrum is *bounded* and always contains an *absolutely continuous part.* An additional discrete (point) spectrum is also allowed but a singularly continuous spectrum is left out of our consideration.

Hence the spectral representation

$$G(z)=\int \frac{w(x)}{z-x}\,\mathrm{d}x \tag{2.1}$$

is possible and the spectral function $w(x)$ is decomposed into two parts; the non-negative Lebesgue integrable function with the bounded and non-empty support (absolutely continuous part), and the assembly (or null) of δ functions corresponding to a discrete spectrum. In the present theory we are interested in the *asymptotic* properties of the recursion method. As will be seen later in § 4.3 they are not affected by a discrete spectrum, and so we leave it out of account for the present. Thus it is hereafter assumed that $w(x)$ consists of an absolutely continuous spectrum only, i.e. its support is composed of line segments on the real axis.

We can generate the infinite series of states

$$|0\rangle, H|0\rangle, H^2|0\rangle, H^3|0\rangle, \ldots, H^n|0\rangle, \ldots$$

which are linearly independent of one another since $w(x)$ contains a continuous spectrum. Thus the following orthonormalised basis set of infinite dimension, say W, can be constructed by the orthonormalisation of Schmidt

$$W=\{|0\rangle, |1\rangle, |2\rangle, |3\rangle, \ldots, |n\rangle, \ldots\}.$$

We intend to have the (semi-infinite) matrix representation of H in this basis, and then to calculate $G(z)$. It is obvious that the nth ket is written as

$$|n\rangle = p_n(H)|0\rangle \tag{2.2}$$

where $p_n(\,.\,)$ is a polynomial of degree n. It is familiar that the matrix representation of H is tridiagonal, and the following recurrence relation holds:

$$b_n|n+1\rangle=(H-a_n)|n\rangle - b^*_{n-1}|n-1\rangle \tag{2.3}$$

where a_n and b_n are the recursion coefficients and are the diagonal and subdiagonal elements respectively:

$$a_n=\langle n|H|n\rangle \qquad b_n=\langle n+1|H|n\rangle. \tag{2.4}$$

In general b_n is complex while a_n is real, but the phase of b_n (i.e. the phase of $|n+1\rangle$) can be chosen arbitrarily, so we hereafter let b_n be real and positive (non-zero). Then it follows that $p_n(x)$ is a polynomial with real coefficients. The expression for $G(z)$ by use of the recursion coefficients is also familiar:

$$G(z)=(z-a_0-b_0^2/\{z-a_1-b_1^2/[z-a_2-b_2^2/(z-\ldots)]\})^{-1}. \tag{2.5}$$

We next introduce the spectral representation of H

$$H=\int |x\rangle x\langle x|N(x)\,\mathrm{d}x \tag{2.6}$$

where $N(x)$ is the density of states and the unit operator is written as $I=\int |x\rangle\langle x|N(x)\,\mathrm{d}x$. Note that the orthonormalisation relation between the $|x\rangle$ is written as $\langle x|x'\rangle=\delta(x-x')/N(x)$. It is readily seen that the spectral function in (2.1) is given as $w(x)=N(x)|\langle x|0\rangle|^2$ and $w(x)$ is normalised as

$$\int w(x)\,\mathrm{d}x=\langle 0|0\rangle=1.$$

Hereafter the ket indicated by the letter x denotes the eigenstate whose eigenenergy is x, while a numeral or the letter m or n represents the basis state in W.

From the orthonormalisation relation between $|n\rangle$ we have

$$\langle m|n\rangle=\int p_m(x)p_n(x)w(x)\,\mathrm{d}x=\delta_{mn}. \tag{2.7}$$

Consequently the sequence of polynomials $p_n(x)$ constitutes the system of orthonormal polynomials whose associated weight is $w(x)$. The recurrence relation for $p_n(x)$ is apparent from (2.2) and (2.3). The function $w(x)$, which is the spectral function of $G(z)$ and at the same time is the weight function corresponding to the orthonormal polynomials $p_n(x)$, is often called the *band* throughout this paper.

We introduce the orthogonal (not normalised) polynomial $P_n(x)$ whose leading coefficient is unity, and let its square norm be κ_n

$$P_n(x)=x^n+\ldots=\kappa_n p_n(x) \tag{2.8}$$

$$\kappa_n=\|P_n(.)\|\equiv\left(\int w(x)[P_n(x)]^2\,\mathrm{d}x\right)^{1/2}=\prod_{j=0}^{n-1} b_j. \tag{2.9}$$

As will be seen later, $P_n(x)$ is more convenient than $p_n(x)$ in the present theory, and an energy argument x is to be extended to the complex plane. The analytic continuation of $P_n(x)$ to the complex argument is trivial since it is a polynomial. Hereafter the letter z is used to denote a point in the complex energy plane, while x is a point on the real axis. When z is used, the infinity is also regarded as an ordinary point. We will use $P_n(z)$ in many cases, while $p_n(x)$ or $P_n(x)$ appears occasionally.

Regarding $P_n(z)$ the recurrence identity comes to have a form

$$P_{n+1}(z)=(z-a_n)P_n(z)-b_{n-1}^2P_{n-1}(z). \tag{2.10}$$

This recurrence equation has two linearly independent (concerning n) solutions; one is $P_n(z)$ and the second-kind function $Q_n(z)$ defined by

$$Q_n(z)=\int\frac{w(x)}{z-x}P_n(x)\,\mathrm{d}x \tag{2.11}$$

is introduced as the other. Note that infinity is a pole of multiplicity n for $P_n(z)$, while it is a zero of multiplicity $n+1$ for $Q_n(z)$, i.e. the Laurent and the Taylor series at infinity are given as

$$P_n(z) = z^n + \ldots \qquad Q_n(z) = \kappa_n^2/z^{n+1} + \ldots. \tag{2.12}$$

We also introduce the analytic function, $g_n(z)$, defined by the following infinite continued fraction:

$$g_n(z) = (z - a_n - b_n^2/\{z - a_{n+1} - b_{n+1}^2/[z - a_{n+2} - b_{n+2}^2/(z - \ldots)]\})^{-1} \tag{2.13}$$

which has the same analyticity as $G(z)$ in the sense that in the physical sheet it is holomorphic with no zeros except infinity (a simple zero), and its imaginary part has an opposite sign to Im z. Note that $Q_0(z) = g_0(z) = G(z)$. It is easy to show that

$$Q_n(z) = \kappa_n^2 \prod_{j=0}^{n} g_j(z) \tag{2.14}$$

from the fact that the right-hand side of (2.14) satisfies the recurrence relation (2.10).

The case where an energy is real with infinitesimal imaginary part, $z = x \pm \mathrm{i}0$, will also be necessary. In this case it suits our convenience to represent $g_n(x \pm \mathrm{i}0)$ by its absolute value and argument

$$g_n(x \pm \mathrm{i}0) = \bar{g}_n(x) \exp(\mp \mathrm{i}\theta_n(x)). \tag{2.15}$$

It is obvious that $\theta_n(+\infty) = 0$, $\theta_n(-\infty) = \pi$ and $0 \leqslant \theta_n(x) \leqslant \pi$, but $\theta_n(x)$ is not necessarily monotone non-increasing. The second-kind function is then expressed from (2.14) as

$$Q_n(x \pm \mathrm{i}0) = \bar{Q}_n(x) \exp(\mp \mathrm{i}\Theta_{n+1}(x)) \tag{2.16}$$

$$\bar{Q}_n(x) = \kappa_n^2 \prod_{j=0}^{n} \bar{g}_j(x) \qquad \Theta_n(x) = \sum_{j=0}^{n-1} \theta_j(x) \qquad 0 \leqslant \Theta_n(x) \leqslant n\pi. \tag{2.17}$$

The value of $P_n(x)$, which is real, can be written as

$$\begin{aligned} P_n(x) &= (\bar{Q}_n(x)/\pi w(x)) \sin \Theta_{n+1}(x) \\ &= \left(\sin \theta_n(x) \prod_{j=0}^{n-1} \bar{g}_j(x) \right)^{-1} \sin \Theta_{n+1}(x). \end{aligned} \tag{2.18}$$

Here the first equation is obtained from (2.11) and the following well known identity is used for the second one

$$P_{n+1}(z)Q_n(z) - P_n(z)Q_{n+1}(z) = \kappa_n^2.$$

Note that the expressions (2.18) are not valid at the band edges, nor in general at the branch points of $G(z)$ whose cuts extend to the unphysical sheet, since they are also the branch points of $Q_n(z)$ and thus expression (2.16) is inadequate there.

Finally we refer briefly to the Szegö theory which, as previously mentioned, can be applied to the single-band case. We can assume, without restricting the generality, that the band is spread between -1 and 1. Then according to the Szegö theory (Szegö 1958) if the weight function $w(x)$ satisfies the Szegö condition

$$\int_{-1}^{1} (1 - x^2)^{-1/2} \ln w(x)\, \mathrm{d}x > -\infty$$

then the corresponding orthogonal polynomial $P_n(z)$ satisfies the following two limit identities:

$$\lim_{n\to\infty} (P_n(z))^{1/n} = \lim_{n\to\infty} (P_{n+1}(z)/P_n(z)) = \tfrac{1}{2}[z+(z^2-1)^{1/2}] \qquad \text{for } z \notin [-1,1] \tag{2.19}$$

where both the two roots have their principal values z as $z\to\infty$. It is known that the Szegö condition is a *sufficient* (not necessary) condition for the limit identity (2.19). Note that the limit function is the one which maps the exterior of the line segment $[-1, 1]$ conformally on the exterior of the circle of radius $\frac{1}{2}$. When the second limit identity is substituted into the recurrence relation (2.10), and the Laurent expansion at infinity is taken, then it is straightforward to obtain the well known convergence of the recursion coefficients.

3. Exterior mapping problem

In the present theory we treat a set in the complex plane and a conformal mapping of a certain kind. The following conventions of notations and terminologies, etc, are used throughout this paper.

(i) *Notations.* When a set S is given in the complex plane, then its complement and its boundary are denoted by $C[S]$ and ∂S, respectively. We mean by $\Pi_n(z)$ a polynomial of degree n whose leading coefficient is unity, i.e. $\Pi_n(z) = z^n + \ldots$.

When an arbitrary function $f(z)$, which is often a polynomial, is given, the maximum of its absolute value in a closed set S is denoted by $M(f; S)$, i.e. $M(f; S) = \max_{z\in S} |f(z)|$.

(ii) *Root.* The nth root of $\Pi_n(z)$ is often taken. This root is chosen to have the principal value such that $(\Pi_n(z))^{1/n}/z = 1$ at infinity.

(iii) *Continuum.* A continuum is originally defined (see Hille 1959) as being a non-empty closed set which cannot be separated into the union of two disjoint non-empty closed sets. The case of a single point is excluded. A line segment belongs to a continuum.

In the present theory we usually treat a *bounded continuum whose complement is simply connected,* which is hereafter referred to as a *continuum* for simplicity. We use the symbol E to denote a continuum under consideration. In many cases the union of disjoint continua is also considered, where the union is denoted by E, and its kth component continuum is indicated by e_k, i.e. $E = e_1 + e_2 + e_3 + \ldots$, where $e_i \cap e_j = 0$ for $i \neq j$. Note that $C[E]$ is open since E is closed, and $C[E]$ contains infinity as an interior point since E is bounded.

(iv) *Exterior mapping function* (EMF). Suppose that E is a continuum (in the above sense). Then there exists the analytic function $F(z)(= z + \ldots$ as $z\to\infty)$, such that it maps $C[E]$ conformally on the exterior of a circle centred at the origin. The function $F(z)$ is unique and is called the exterior mapping function (EMF) (Hille 1962, p 339). The radius of the circle is called the exterior mapping radius. In this definition it is necessary that $C[E]$ is simply connected, but in the present theory this EMF is generalised to include the case where E is a union of disjoint continua and thus $C[E]$ is multiply connected.

First of all, we consider the problem of the two-dimensional electrostatic potential in the system of conductors. Suppose that the finite number, say m, of solid conductors are distributed with no contacts in the two-dimensional plane, and electric charges can move freely from one conductor to another, i.e. the potentials of all conductors are kept to be equal to one another. Each conductor is evidently regarded as a continuum in the complex plane, and the system of conductors forms a union of disjoint continua and so is denoted by E whose kth component conductor is e_k. The case of a single conductor is not excluded.

Then we assume that continuous charge 2π is given on E, and introduce the complex potential (Panofsky and Phillips 1962), defined in the usual manner where a point charge q, located at z_0, causes the complex potential $f(z) = -(q/2\pi)\ln(z-z_0)$. The curves $\operatorname{Re} f(z) = \text{constant}$ and $\operatorname{Im} f(z) = \text{constant}$ give the equipotential curves and the streamlines (lines of electrical forces) respectively. The charge distribution is unique, and thus the complex potential (analytic function), $\phi(z; E)$, which is defined in $C[E]$, exists under the condition that $\phi(z; E) = -\ln z + O(1/z)$ as $z \to \infty$. The point infinity is a branch point of $\phi(z; E)$. In the general case where E is a union of two or more disjoint continua, $\phi(z; E)$ has the other multivalued property. When z is moved round counterclockwise along a closed curve which surrounds one component continuum only, say e_k, then $\phi(z; E)$ is increased by $-iq_k$, q_k being the charge on e_k. Thus the multivalued property appears in $\operatorname{Im} \phi(z; E)$ only and in every case $\operatorname{Re} \phi(z; E)$ is single valued. When z is on the surface of conductors ∂E, the equality $\operatorname{Re} \phi(z \in \partial E; E) = V(E)$ holds, $V(E)$ being the electrostatic potential of E.

In the present theory the function defined for $z \in C[E]$ by

$$\Phi(z; E) = \exp[-\phi(z; E)] \tag{3.1}$$

is more convenient than $\phi(z; E)$. The absolute value of $\Phi(z; E)$ is single valued in $C[E]$, although its argument is multivalued. We make the branch cuts for $\Phi(z; E)$ as follows: let E^c be the set of points on the streamlines passing through the saddle points of the electrostatic potential (see figure 1), then we cut the domain $C[E]$ along E^c, which is a union of arcs, and let $E^* = E \cup E^c$. Note that E^c is unique. The set E^* is a bounded continuum, whose complement $C[E^*]$ is simply connected. The analytic function $\Phi(z; E)$ is univalent and meromorphic in $C[E^*]$ with a singularity at infinity (a simple pole) only, and has the Laurent series as

$$\Phi(z; E) = z + c_0 + c_1/z + \ldots.$$

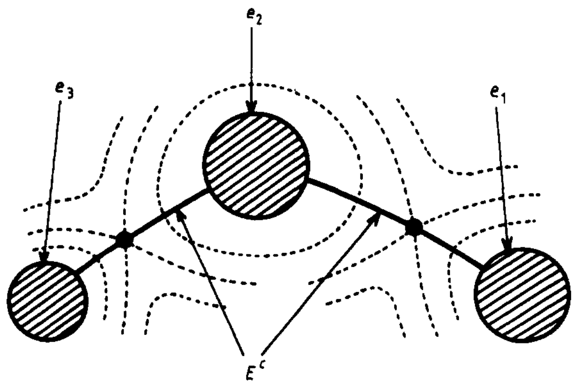

Figure 1. Branch cuts (E^c: full lines) for $\Phi(z; E)$. E is composed of e_1, e_2 and e_3. E^c is given by the streamlines passing through the saddle points (●) of the potential. The broken curves are the equipotential curves.

The equipotential curves and the streamlines are now given by $|\Phi(z; E)| = \text{constant}$ and $\arg \Phi(z; E) = \text{constant}$, respectively. On the boundary of E, we have $|\Phi(z \in \partial E; E)| = \gamma(E) = e^{-V(E)}$. The quantity $\gamma(E)$ is called the logarithmic capacity of E (Hille 1962).

Let us examine what mapping is obtained by the function $\zeta = \Phi(z; E)$. When z moves along ∂E, then ζ evidently moves on the circle: $|\zeta| = \gamma(E)$, while the locus for $z \in E^c$ is on the line segments which start straightforwards out of this circle (see figure 2). Thus we can see that $\Phi(z; E)$ maps $C[E^*]$ conformally on the exterior of *the disc with whiskers*, which is the union of the disc of radius $\gamma(E)$ and the line segments, the latter of which are the image of E^c. For simplicity we hereafter call such a function a generalised exterior mapping function (EMF), and mean the above situation by the statement that $\Phi(z; E)$ *is the* EMF *such that* $E \to \gamma(E)$. The limit function in the limit identity (2.19) by Szegö is the EMF such that $[-1, 1] \to \frac{1}{2}$.

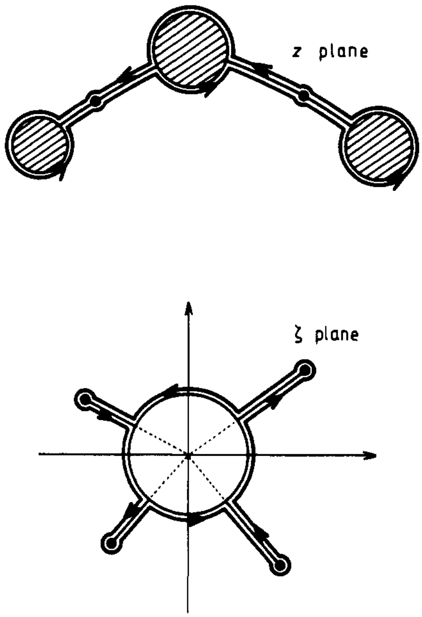

Figure 2. Schematic depiction of a conformal mapping by the EMF: $\zeta = \Phi(z; E)$. The saddle points and their images are indicated by ●.

The radius of the disc which equals the logarithmic capacity should be called the generalised exterior mapping radius, and is also equal to the quantities which have other names according to their definitions: transfinite diameter and Tchebycheff constant (see appendix 1). Hereafter we use the term *transfinite diameter* to denote $\gamma(E)$.

Now we can have a fundamental theorem as concerns the limit of the nth root of a certain family of polynomials (see Walsh 1956).

Theorem 1. Let $\{\Pi_n(z)\}$ be a sequence of polynomials. Suppose that

$$\lim_{n\to\infty} [M(\Pi_n; E)]^{1/n} = \gamma(E) \tag{3.2}$$

and all zeros of $\Pi_n(z)$ are bounded, then

$$\lim_{n\to\infty} [\Pi_n(z)]^{1/n} \equiv \Phi(z; E) \qquad \text{for } z \in C[E^+] \tag{3.3}$$

where E^+ is a bounded continuum, such that it contains E^*, all zeros of $\Pi_n(z)$ are located in E^+, and $C[E^+]$ is simply connected.

Note that the right-hand side of (3.3) is analytic in $C[E]$ (although it is not necessarily single valued), and thus the analytic continuation is possible as far as the left-hand side can be defined. The proof of theorem 1 is as follows. Consider the function $\Pi_n(z)/(\Phi(z;E))^n$, defined in $C[E]$, where it is holomorphic and its absolute value is single valued. By the maximum principle we have

$$|\Pi_n(z)|/|\Phi(z;E)|^n \leqslant M(\Pi_n/\Phi^n;\partial E) = M(\Pi_n;E)/(\gamma(E))^n \qquad \text{for } z\in C[E].$$

Let its nth root be $f_n(z)$

$$f_n(z) = (\Pi_n(z))^{1/n}/\Phi(z;E) \tag{3.4}$$

then $f_n(z)$ is holomorphic and single valued in $C[E^+]$ even at infinity (not in $C[E^*]$ if the zero of $\Pi_n(z)$ exists in $C[E^*]$) and

$$f_n(\infty) = 1 \tag{3.5}$$

$$|f_n(z)| \leqslant [M(\Pi_n;E)]^{1/n}/\gamma(E) \qquad \text{for } z\in C[E^+]. \tag{3.6}$$

Thus from the hypothesis $f_n(z)$ is uniformly bounded in $C[E^+]$, and consequently $\{f_n(z)\}$ is a normal family in $C[E^+]$ (see Hille 1962, p 235). We can then find a subsequence which converges to a limit function, which takes the value unity at infinity, and whose absolute value in $C[E^+]$ is not greater than unity from (3.6) and the hypothesis. So it is identically equal to unity by the maximum principle, which applies to every limit function. Therefore it is concluded that

$$\lim_{n\to\infty} f_n(z) \equiv 1 \qquad \text{for } z\in C[E^+]$$

and the proof is completed.

It is to be noted that this proof is also valid when equations (3.5) and (3.6) are replaced by the following limit relations:

$$\lim_{n\to\infty} f_n(\infty) = 1 \tag{3.7}$$

$$\limsup_{n\to\infty} |f_n(z)| \leqslant 1 \qquad \text{for } z\in\partial E. \tag{3.8}$$

There exist several kinds of polynomials which satisfy the hypothesis of this theorem. One of the most important is the Tchebycheff polynomial, $T_n(z;E) = z^n + \ldots$ (see appendix 1), which is defined as minimising among $\Pi_n(z)$ the maximum of its absolute value in E.

4. Asymptotic forms of orthogonal polynomials

In the present theory the multiband case is treated in general. The support of the band $w(x)$ is then a union of disjoint continua, each of which is a line segment on the real axis. Let m be the number of comonent line segments, then the support E is written as

$$E = e_1 + e_2 + e_3 + \ldots + e_m$$
$$e_k = [B_k, A_k] \qquad k = 1, 2, \ldots, m$$
$$B_m < A_m < \ldots < B_2 < A_2 < B_1 < A_1.$$

Note that A_k and B_k are given in descending order.

The orthogonal polynomial and other related functions have been introduced in § 2, where their exprressions contain only one argument, x or z. They are, of course, functions not only of x or z but also of the band, and so the support of the band is hereafter included in the argument, i.e. the notations such as $P_n(z; E)$, $Q_n(z; E)$, etc, are used. Note that they also depend on the band shape, although it is not explicitly written. On the contrary, the EMF, $\Phi(z; E)$, which has been introduced in § 3 and is expressed in the same form, depends on the support only. Here and hereafter the term *band shape* is used to specify the variety of weight functions (spectral structures) with the same support.

4.1. *The Geronimus condition*

Theorem 1 is applicable to the orthogonal polynomials, when the band $w(x)$ satisfies the condition

$$\lim_{\delta\to+0} \delta^{1/2} \ln a(\delta) = 0 \qquad a(\delta) = \inf_{[x,x+\delta]\subset E} \int_x^{x+\delta} w(x)\,\mathrm{d}x. \tag{4.1}$$

This condition should be named after Geronimus (1960).

Theorem 2. Suppose that the weight $w(x)$ satisfies the Geronimus condition (4.1), and let $P_n(x; E)$ be the corresponding orthogonal polynomial with a leading coefficient unity, then we have

$$\lim_{n\to\infty} (P_n(z; E))^{1/n} \equiv \Phi(z; E) \qquad \text{for } z \in C[E^*] \tag{4.2}$$

$$\lim_{n\to\infty} (\kappa_n(E))^{1/n} = \lim_{n\to\infty} (M(P_n(\cdot\,; E); E))^{1/n} = \gamma(E). \tag{4.3}$$

It is obvious that $E^* = [B_m, A_1]$. It is well known that all zeros of $P_n(z; E)$ are located on E^* (not necessarily on E), i.e. they are bounded, and we can take $E^+ = E^*$.

We refer to the minimal properties of the orthogonal $[P_n(z; E)]$ and the Tchebycheff $[T_n(z; E)]$ polynomials. They minimise among $\Pi_n(z)$, the square norm and the maximum of the absolute value in E, respectively. From these properties we have

$$\kappa_n(E) = \|P_n(\cdot\,; E)\| \leq \|T_n(\cdot\,; E)\| \leq M(T_n(\cdot\,; E); E) \leq M(P_n(\cdot\,; E); E) \tag{4.4}$$

where the well known relation $\|f(\cdot)\| \leq M(f; E)$, is used. We know that $\lim_{n\to\infty} (M(T_n(\cdot\,; E); E))^{1/n} = \gamma(E)$ (see appendix 1) and thus we can complete the proof if we have the limit relation

$$\liminf_{n\to\infty} [\kappa_n / M(P_n(\cdot\,; E); E)]^{1/n} \geq 1 \tag{4.5}$$

which is nothing but the convergence to unity since the superior limit is not greater than unity from (4.4).

Geronimus (1960, p 151) showed that the condition (4.1) is sufficient (not necessary) for the relation (4.5) in the single-band case. His argument did not explicitly include the multiband case, but can be easily extended. Suppose that $P_n(x; E)$ attains the maximum of its absolute value in E at $x_0 \in e_k$, and let $M_n = M(P_n(\cdot\,; E); E)$ for simplicity. Then the Markoff inequality (see Schaeffer 1941) written as

$$M(\Pi'_n(x); [-1, 1]) \leq n^2 M(\Pi_n(x); [-1, 1])$$

where $\Pi_n(x)$ is arbitrary with real coefficients and $\Pi_n'(x)$ is its derivative, leads to the relation

$$|P_n(x;\, E)| \geq \tfrac{1}{2} M_n$$

for $|x - x_0| \leq w_k/4n^2$ and $x \in e_k$, where $w_k = A_k - B_k$. Hence we may obtain

$$(\kappa_n/M_n)^2 \geq \inf_{[x,x+w_k/4n^2]\subset e_k} \int_x^{x+w_k/4n^2} w(x)\,\mathrm{d}x.$$

Now it is obvious that the condition (4.1) is sufficient for (4.5), i.e. the proof of theorem 2 is completed.

Concerning the second-kind function we have the following theorem.

Theorem 3. Suppose that the Geronimus condition is satisfied, then

$$\lim_{n\to\infty} [Q_n(z;\, E)]^{1/(n+1)} \equiv [\gamma(E)]^2 [\Phi(z;\, E)]^{-1} \qquad \text{for } z \in C[E^*] \tag{4.6}$$

where the root is so taken as to have the same argument as $1/z$ at infinity (see (2.12)).

Proof. Note that the zeros of $Q_n(z;\, E)$ are located at infinity (multiplicity $n+1$) and on E^c. We let

$$f_n(z) = [Q_n(z;\, E)]^{1/(n+1)} \Phi(z;\, E)/[\gamma(E)]^2$$

and then intend to prove

$$\lim_{n\to\infty} f_n(z) \equiv 1 \qquad \text{for } z \in C[E^*].$$

We see that $f_n(z)$ is holomorphic and single valued in $C[E^*]$ and

$$f_n(\infty) = [\kappa_n(E)]^{2/(n+1)}/[\gamma(E)]^2 \xrightarrow[n\to\infty]{} 1$$

while $|f_n(z)|$ is single valued in $C[E]$. Let E_ε be the region surrounded by the equipotential curves outside E, given by $E_\varepsilon = \{z \,|\, |\Phi(z;\, E)| \leq \gamma(E) + \varepsilon\}$, where ε is an arbitrary (small) positive constant. It is obvious that E_ε is a union of disjoint continua (or a single continuum), and contracts to E as $\varepsilon \to +0$. The EMF such that $E \to \gamma(E)$ is also the EMF such that $E_\varepsilon \to \gamma(E) + \varepsilon$. From (2.11) we have

$$|Q_n(z;\, E)| \leq M(P_n(\cdot\,;\, E);\, E) \Big/ \min_{z\in\partial E_\varepsilon,\, x\in E} |z - x| \qquad \text{for } z \in \partial E_\varepsilon. \tag{4.7}$$

As concerns the lower bound of $|z - x|$, where $z \in \partial E_\varepsilon$ and $x \in E$, we can find an adequate positive number c independent of ε, such that

$$\min_{z\in\partial E_\varepsilon,\, x\in E} |z - x| \geq c\varepsilon^2.$$

Substitute this into (4.7) and take the $(n+1)$th root. Then we have

$$\limsup_{n\to\infty} |f_n(z)| \leq 1 + \varepsilon/\gamma(E) \qquad \text{for } z \in \partial E_\varepsilon.$$

Since ε is arbitrary we have

$$\limsup_{n\to\infty} |f_n(z)| \leq 1 \qquad \text{for } z \in \partial E.$$

Hence theorem 3 is proved by the same argument as the proof of theorem 1 (refer to (3.7) and (3.8)).

As is mentioned before, the Geronimus condition (4.1) is only a *sufficient* (not necessary) condition for theorems 2 and 3. Thus it can be made less restrictive, but no further considerations are given in this paper. At least this condition is satisfactory unless we treat the spectrum which vanishes very singularly at the band edges or inside the band. Hereafter it is assumed without notice that the band shape satisfies the Geronimus condition.

4.2. *Explicit form of* EMF

Our next problem is to ascertain the EMF such that $E \to \gamma(E)$. It is obvious that there exist $m-1$ saddle points of the equipotential curves, each of which appears once in each energy range of the band gaps, i.e. let the saddle points be $s_1, s_2, \ldots, s_{m-1}$ in descending order, then $A_{k+1} < s_k < B_k$.

It is easier to find the complex potential $\phi(z; E)$ than the EMF. From the general properties of the complex potential, we can see that it maps the upper half of the z plane conformally on the open degenerate polygon as is shown in figure 3. The quantity q_k is the charge distributed on e_k. Such a conformal mapping is known as the Schwarz(-Christoffel) transformation (Panofsky and Phillips 1962) and is written as

$$\phi(z; E) = -\int^z \left(\prod_{k=1}^{m-1} (z-s_k)\right)\left(\prod_{k=1}^{m} (z-A_k)(z-B_k)\right)^{-1/2} \mathrm{d}z \tag{4.8}$$

where the argument of the integrand and the integration constant are taken such that $\phi(z; E)$ behaves like $-\ln z$ as $z \to \infty$. Note that the coordinates of s_k should be so chosen that all vertical lines connecting A'_k to B'_k in figure 3 are aligned with one another.

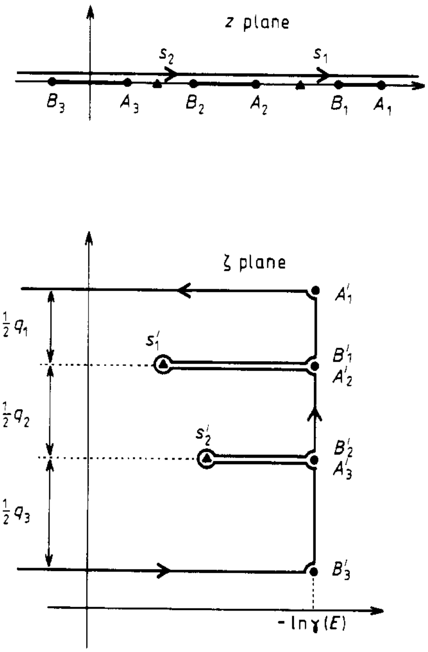

Figure 3. Schematic depiction of a conformal mapping by the complex potential: $\zeta = \phi(z; E)$. The points A'_k, B'_k and s'_k in the ζ plane correspond to A_k, B_k and s_k in the z plane, respectively. The three-band case is shown.

From (4.8) the following relations are obtained, where in order to simplify the equations we use the real function $X(x; E)$ defined on the real axis as

$$X(x; E) = \left(\prod_{k=1}^{m-1} (x - s_k)\right)(R(x; E))^{-1}$$
$$R(x; E) = \left|\prod_{k=1}^{m} (x - A_k)(x - B_k)\right|^{1/2}. \tag{4.9}$$

(i) Impose the alignment of the vertical lines in figure 3, i.e. the equality of the potentials of component conductors

$$\phi(A_{k+1} + \mathrm{i}0; E) = \phi(B_k + \mathrm{i}0; E) \qquad k = 1, 2, \ldots, m-1$$

then we have

$$\int_{A_{k+1}}^{B_k} X(x; E)\,\mathrm{d}x = 0 \qquad k = 1, 2, \ldots, m-1. \tag{4.10}$$

Through this equation s_k is determined as a function of A_k and B_k. We see that s_k $(k = 1, 2, \ldots, m-1)$ are the $m-1$ roots of the algebraic equation of degree $m-1$,

$$\prod_{k=1}^{m-1} (x - s_k) = x^{m-1} + c_{m-2}x^{m-2} + c_{m-1}x^{m-1} + \ldots + c_1 x + c_0 = 0 \tag{4.11}$$

where the coefficients c_i $(i = 0, 1, \ldots, m-2)$ are given by the solutions of the linear simultaneous equation

$$\sum_{i=0}^{m-2} F_{ji} c_i = -F_{j,m-1} \qquad j = 1, 2, \ldots, m-1$$
$$F_{ji} = \int_{A_{j+1}}^{B_j} x^i / R(x; E)\,\mathrm{d}x. \tag{4.12}$$

(ii) Concerning the charge q_k distributed in e_k, which is a function of E only, we have

$$\phi(A_k + \mathrm{i}0; E) - \phi(B_k + \mathrm{i}0; E) = \mathrm{i}q_k/2 \qquad k = 1, 2, \ldots, m$$

and it follows that

$$q_k = 2\int_{B_k}^{A_k} |X(x; E)|\,\mathrm{d}x \qquad k = 1, 2, \ldots, m. \tag{4.13}$$

Note that equation (4.13) is composed of m equations, but one of them is redundant since

$$\sum_{k=1}^{m} q_k = 2\pi. \tag{4.14}$$

(iii) The transfinite diameter $\gamma(E)$ can be calculated by

$$\ln \gamma(E) = -\int_{A_1}^{\infty} \left(X(x; E) - \frac{1}{x - A_1 + 1}\right)\mathrm{d}x. \tag{4.15}$$

(iv) Finally note that the derivative of the argument of the EMF at $z = x \pm \mathrm{i}0$ can be written by $X(x; E)$ as

$$\frac{\mathrm{d}}{\mathrm{d}x}[\arg \Phi(x \pm \mathrm{i}0; E)] = \begin{cases} \mp|X(x; E)| & x \in E \\ 0 & \text{otherwise.} \end{cases} \tag{4.16}$$

4.3. Limit relations of recursion coefficients

First of all it is readily seen from (2.9) and (4.3) that

$$\lim_{n\to\infty}\left(\prod_{j=0}^{n-1} b_j\right)^{1/n} = \gamma(E) \tag{4.17}$$

which is a generalisation of the convergence of b_n in the single-band case. This relation indicates the limit of the geometric mean, while in the following the relations associated with the limits of the arithmetic means are given.

The analytic function $D_n(z; E)$, which is holomorphic in $C[E^*]$, is introduced:

$$D_n(z; E) = P_n(z; E)/(\Phi(z; E))^n. \tag{4.18}$$

This satisfies

$$\begin{aligned} &D_n(\infty; E) = 1 \\ &\lim_{n\to\infty} [D_n(z; E)]^{1/n} \equiv 1 \qquad \text{for } z \in C[E^*]. \end{aligned} \tag{4.19}$$

We define the coefficients d_{ni} and λ_i ($i = 1, 2, 3, \ldots$) by the following Taylor expansions:

$$-\ln D_n(z; E) = d_{n1}/z + d_{n2}/z^2 + d_{n3}/z^3 + \ldots \tag{4.20}$$

$$\begin{aligned} -\ln(\Phi(z; E)/z) &= \phi(z; E) + \ln z \\ &= \lambda_1/z + (\lambda_2/2)/z^2 + (\lambda_3/3)/z^3 + \ldots. \end{aligned} \tag{4.21}$$

Note that the λ_i also depend only on E. From the limit identity (4.19) d_{ni} has the limit property

$$\lim_{n\to\infty} ((1/n)d_{ni}) = 0 \qquad i = 1, 2, 3, \ldots.$$

We rather use the quantity $\Delta d_{ni} = d_{n+1,i} - d_{ni}$, which satisfies

$$\frac{1}{n}\sum_{j=0}^{n-1} \Delta d_{ji} = \frac{1}{n}(d_{ni} - d_{0i}) \xrightarrow[n\to\infty]{} 0. \tag{4.22}$$

Let us examine the Taylor series (at infinity) of the function

$$f_n(z) = P_{n+1}(z; E)/(zP_n(z; E)) = D_{n+1}(z; E)\Phi(z; E)/(zD_n(z; E)).$$

From the recurrence identity (2.10) of $P_n(z; E)$ we have

$$f_n(z) = 1 - [a_n/z + b_{n-1}^2/z^2 + a_{n-1}b_{n-1}^2/z^3 + (a_{n-1}^2 + b_{n-2}^2)b_{n-1}^2/z^4 + \ldots] \tag{4.23}$$

while by substituting (4.20) and (4.21)

$$\ln f_n(z) = -[(\lambda_1 + \Delta d_{n1})/z + (\lambda_2/2 + \Delta d_{n2})/z^2 + (\lambda_3/3 + \Delta d_{n3})/z^3 + \ldots]. \tag{4.24}$$

Comparing the $1/z$ terms of $\ln f_n(z)$ from (4.23) and in (4.24), we have $\lambda_1 + \Delta d_{n1} = a_n$, and hence by (4.22),

$$\lambda_1 = \lim_{n\to\infty}\left(\frac{1}{n}\sum_{j=0}^{n-1} a_j\right) \tag{4.25}$$

which is a generalisation of the convergence of a_n in the single-band case.

Using the terms of higher powers of $1/z$ from (4.23) and in (4.24), a set of limit relations of the recursion coefficients can be obtained successively after the straightforward but tedious calculations

$$
\begin{aligned}
&\lambda_1 = \langle\langle a_0 \rangle\rangle \\
&\tfrac{1}{2}\lambda_2 = \langle\langle b_0^2 \rangle\rangle + \tfrac{1}{2}\langle\langle a_1^2 \rangle\rangle \\
&\tfrac{1}{3}\lambda_3 = \langle\langle (a_0 + a_1) b_0^2 \rangle\rangle + \tfrac{1}{3}\langle\langle a_1^3 \rangle\rangle \\
&\tfrac{1}{4}\lambda_4 = \langle\langle b_0^2 b_1^2 \rangle\rangle + \tfrac{1}{2}\langle\langle b_1^4 \rangle\rangle + \langle\langle (a_1^2 + a_1 a_2 + a_2^2) b_1^2 \rangle\rangle + \tfrac{1}{4}\langle\langle a_2^4 \rangle\rangle \\
&\tfrac{1}{5}\lambda_5 = \langle\langle (a_0 + 2a_1 + a_2) b_0^2 b_1^2 \rangle\rangle + \langle\langle (a_1 + a_2) b_1^4 \rangle\rangle + \langle\langle (a_1^3 + a_1^2 a_2 + a_1 a_2^2 + a_2^3) b_1^2 \rangle\rangle + \tfrac{1}{5}\langle\langle a_2^5 \rangle\rangle \\
&\tfrac{1}{6}\lambda_6 = \langle\langle b_0^2 b_1^2 b_2^2 \rangle\rangle + \langle\langle (b_1^2 + b_2^2) b_1^2 b_2^2 \rangle\rangle + \tfrac{1}{3}\langle\langle b_2^6 \rangle\rangle + \langle\langle (a_1^2 + 2a_1 a_2 + a_1 a_3 + 3a_2^2 \\
&\qquad + 2a_2 a_3 + a_3^2) b_1^2 b_2^2 \rangle\rangle + \langle\langle (\tfrac{3}{2}a_2^2 + 2a_2 a_3 + \tfrac{3}{2}a_3^2) b_2^4 \rangle\rangle \\
&\qquad + \langle\langle (a_2^4 + a_2^3 a_3 + a_2^2 a_3^2 + a_2 a_3^3 + a_3^4) b_2^2 \rangle\rangle + \tfrac{1}{6}\langle\langle a_3^6 \rangle\rangle
\end{aligned} \tag{4.26}
$$

etc. Here for simplicity we have used the notation

$$
\langle\langle a_r^p b_s^q \rangle\rangle = \lim_{n\to\infty} \left(\frac{1}{n} \sum_{j=0}^{n-1} a_{j+r}^p b_{j+s}^q \right) \qquad p, q, r, s = 0, 1, 2, 3, \ldots \tag{4.27}
$$

and so on. The first equation in (4.26) is the same as (4.25). Note that $\langle\langle a_0 \rangle\rangle = \langle\langle a_1 \rangle\rangle = \langle\langle a_2 \rangle\rangle = \ldots$, $\langle\langle a_1 b_0^2 \rangle\rangle = \langle\langle a_2 b_1^2 \rangle\rangle = \langle\langle a_3 b_2^2 \rangle\rangle = \ldots$, etc, and that when a_n and b_n are periodic with the same period the right-hand side of (4.27) can be replaced by the average over one period.

The quantities λ_i $(i = 1, 2, 3, \ldots)$ can be expressed by A_k and B_k $(k = 1, 2, \ldots, m)$ as follows. Note that s_k $(k = 1, 2, \ldots, m-1)$ are determined by A_k and B_k through (4.11) and (4.12). By differentiating (4.21), we have

$$
\prod_{k=1}^{m-1} (1 - s_k/z) \left(\prod_{k=1}^{m} (1 - A_k/z)(1 - B_k/z) \right)^{-1/2} = 1 + \lambda_1/z + \lambda_2/z^2 + \lambda_3/z^3 + \ldots
$$

from which the following relations are obtained:

$$
\begin{aligned}
&\lambda_1 = \mu_1 \\
&\lambda_2 = \mu_2 + \tfrac{1}{2}\mu_1^2 \\
&\lambda_3 = \mu_3 + \mu_1 \mu_2 + \tfrac{1}{6}\mu_1^3 \\
&\lambda_4 = \mu_4 + \mu_1 \mu_3 + \tfrac{1}{2}\mu_2^2 + \tfrac{1}{2}\mu_1^2 \mu_2 + \tfrac{1}{24}\mu_1^4 \\
&\lambda_5 = \mu_5 + \mu_1 \mu_4 + \mu_2 \mu_3 + \tfrac{1}{2}\mu_1^2 \mu_3 + \tfrac{1}{2}\mu_1 \mu_2^2 + \tfrac{1}{6}\mu_1^3 \mu_2 + \tfrac{1}{120}\mu_1^5 \\
&\lambda_6 = \mu_6 + \mu_1 \mu_5 + \mu_2 \mu_4 + \tfrac{1}{2}\mu_1^2 \mu_4 + \tfrac{1}{2}\mu_3^2 + \mu_1 \mu_2 \mu_3 + \tfrac{1}{6}\mu_1^3 \mu_3 + \tfrac{1}{6}\mu_2^3 \\
&\qquad + \tfrac{1}{4}\mu_1^2 \mu_2^2 + \tfrac{1}{24}\mu_1^4 \mu_2 + \tfrac{1}{720}\mu_1^6
\end{aligned} \tag{4.28}
$$

etc, where μ_j is defined by

$$
\mu_j = \frac{1}{j} \left(\frac{1}{2} \sum_{k=1}^{m} (A_k^j + B_k^j) - \sum_{k=1}^{m-1} s_k^j \right) \qquad j = 1, 2, 3, \ldots. \tag{4.29}
$$

As mentioned in § 2 the spectrum under consideration has been assumed to have no discrete (δ-functional) part. Here we consider what may happen if an additional discrete spectrum is also taken into account. Suppose that there exists a δ-functional spectrum outside the band, i.e. $w(x)$ has the support (in the sense of the support of the distribution) $\tilde{E} = E + \Delta$, where E is a union of disjoint continua, Δ is a finite (or countable) point set, and $E \cap \Delta = 0$. We can consider the situation where the continuous charge is put on $\tilde{E}$, and also define the complex potential, the EMF of $\tilde{E}$, etc, in the same manner as in § 3. It is obvious that the point set Δ never contains any portion of continuous charge. Therefore the EMF of $\tilde{E}$ is the same as the EMF of E, i.e. the the limit relations obtained in this section are not altered by Δ. That is to say, the asymptotic behaviours of the recursion coefficients are not affected by the discrete spectrum in $w(x)$. No further argument is evidently needed as concerns the discrete spectrum inside the band.

4.4. *Period of asymptotic oscillations*

Although rigorous arguments have been developed until now, we need some speculations in this subsection.

First suppose for simplicity that only one gap exists and the recursion coefficients make periodic oscillations whose period is an integer p

$$a_{p+j} = a_j \qquad b_{p+j} = b_j \qquad \text{for } j = 0, 1, 2, \ldots .$$

Then it is obvious from the definition (2.13) that $g_j(z; E)$ and its argument at $z = x - \mathrm{i}0$, $\theta_j(x; E)$, are also periodic. Using the relation (2.14) and theorem 3, we may obtain

$$\sum_{j=0}^{p-1} \theta_j(x; E) = p \arg \Phi(x + \mathrm{i}0; E). \tag{4.30}$$

Note that the limit $p \to \infty$ is not taken.

From the analyticity of $g_j(z; E)$ one can see that $\theta_j(x; E)$ varies in one of the manners which are schematically shown in figure 4. Let x be in the band gap, then the right-hand side of (4.30) is $pq_1/2$, and so the relation $pq_1/2 = 0 \pmod{\pi}$ must hold. If the cases of two or more gaps are also taken into account then we have

$$pq_k = 0 \pmod{2\pi} \qquad k = 1, 2, \ldots, m \tag{4.31}$$

one of which is redundant (see (4.14)). This is the necessary condition for the completely periodic oscillations with integral period p, and also for the asymptotic periodicity, since the same argument is also valid if the summation in (4.30) is replaced by that over the asymptotic forms of $\theta_j(x; E)$.

Next we consider how the recursion coefficients behave when we can find an integer p which satisfies (4.31). We should refer to the fact that the recursion coefficients a_n and b_n are bounded, and thus they must have convergent subsequences. This fact suggests the conjecture that a_n and b_n make asymptotically oscillating behaviours although it cannot be rigorously proved. The situation where they exhibit irregular variations seems to be physically unnatural, and so we assume that this conjecture is true. Here it is reasonable to say that, when p is the least positive integer which satisfies (4.31), then the recursion coefficieints oscillate asymptotically with period p, not $2p$ or more. The period of the oscillations must be an integral multiple of p. Consider the single-gap case and suppose $q_1 = 2\pi/p$. Assume that q_1 becomes a little larger, $q_1 = 2\pi/p + \varepsilon$, ε being infinitesimally small, then

$$|pq_1| < |(2p)q_1| < |(3p)q_1| < \ldots \qquad \pmod{2\pi}.$$

Thus it is unnatural that the oscillation with period $2p$ or more is more preferable than that with period p.

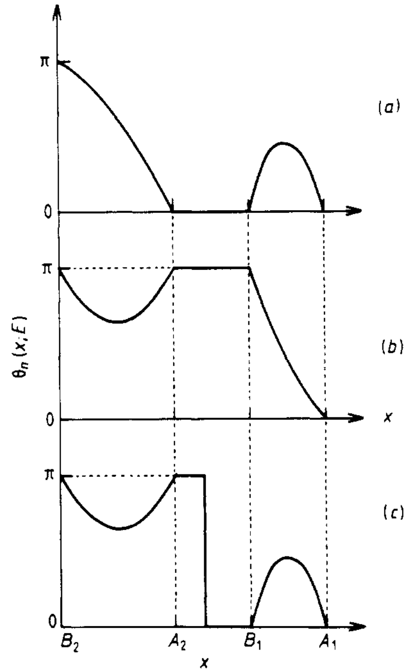

Figure 4. Three types of behaviours of $\theta_n(x; E)$, the argument of $g_n(x-i0; E)$, in the single-gap case. They are classified by the sign of $g_n(x-i0; E)$ when x is in the band gap; it is (*a*) positive, (*b*) negative and (*c*) has a zero in the gap.

Concluding the above arguments the asymptotic recursion coefficients a_n and b_n are written as

$$a_n, b_n \sim S(nq_1, nq_2, \ldots, nq_{m-1}) \tag{4.32}$$

where $S(\ldots)$ stands for a periodic function with period 2π concerning all arguments.

We have considered only the integral period case, i.e. $q_k/2\pi$ being rational, which is not the general situation. It is natural, however, to assume that the asymptotic dependence (4.32) can be extended to the irrational case. In the single-gap case, which seems to be the most important among the multiband cases, the function in (4.32) is reduced to the periodic one with only one argument.

Let us describe our results from a slightly different viewpoint. Consider a two-band case, and suppose $q_1/2\pi = 0.4746$. Then we have $2(q_1/2\pi) = -0.0508 \pmod 1 \sim 0$, which means that the recursion coefficients asymptotically oscillate with period nearly 2. The deviation from 2 is piled up piece by piece, and nearly vanishes (in modulus unity) after $19.7(=1/0.0508)$ repetitions. Thus the asymptotic oscillations look like the mixture of two oscillating subsequences, both of which have period 39.4. In general if $q_1/2\pi$ is near to $\frac{1}{2}$, then two oscillating subsequences with period $|q_1/2\pi - \frac{1}{2}|^{-1}$ will be observed. If $q_1/2\pi$ is near to $\frac{1}{3}$ (or $\frac{2}{3}$), then we have three subsequences with period $|q_1/2\pi - \frac{1}{3}|^{-1}$ (or use $\frac{2}{3}$ instead of $\frac{1}{3}$), and so on.

If we choose a support of a spectrum arbitrarily, then $q_k/2\pi$ is irrational in almost all cases, and we have incommensurate asymptotic oscillations of the recursion coefficients.

4.5. *Comparison with the* TDT *numerical results*

In the TDT paper three figures (Turchi *et al* (1982), figures 2-4) were given to show the asymptotic oscillations of the recursion coefficients in the two-band case. In table 1 the values of the characteristic quantities in the present theory are listed in three cases of the supports corresponding to the three TDT figures. The numbers, e.g. 2-39.4, in the entry *period* in table 1 mean that *two* oscillating subsequences with period 39.4 will be observed. It is readily seen that our results are in good agreement with the numerical results of TDT, if one examines the arithmetic mean of a_n, the geometric mean of b_n and the period of the asymptotic oscillations.

Table 1. The characteristic quantities of the supports treated in numerical work of TDT.

TDT figure	E	λ_1	$\gamma(E)$	$q_1/2\pi$	Period
Figure 2	$[-2, -1.71]+[1.81, 2]$	−0.0712	0.4723	0.4746	2-39.4
Figure 3	$[-2, -0.408]+[0.952, 2]$	−0.0179	0.9391	0.4522	2-20.9
Figure 4	$[-2, 1.1]+[1.5, 2]$	−0.0116	0.9912	0.2711	4-47.4

In figure 18 of their paper, TDT demonstrated the asymptotic oscillations of nearly triple period, which can also be explained by the following evaluation. The support in this case is $[0.5, 1.5]+[2.5, 4.5]+[5, 6]$, and then we have $\lambda_1 = 3.2684$, $\gamma(E) = 1.3372$, $q_1/2\pi = 0.3203$ and $q_2/2\pi = 0.3335$, which leads to *three* subsequences with period 77 by the same discussion as in § 4.4 (note that $q_2/2\pi$ is very close to $\frac{1}{3}$).

5. Properties of the truncated basis

When the recursion method is actually used, the recursion coefficients are computed up to finite order. Then we have the truncated (say, n-dimensional) basis, $W_n = \{|0\rangle, |1\rangle, |2\rangle, \ldots, |n-1\rangle\}$, and the truncated Hamiltonian matrix H_n represented in this basis. Then it is obvious that

$$P_n(x; E) = \det(x - H_n). \tag{5.1}$$

The properties of W_n and H_n are also important when other physical quantities are taken into account in addition to the diagonal element of the resolvent. In this section we consider two problems as concerns their asymptotic features.

The first problem concerns how the zeros of $P_n(x; E)$, i.e. the eigenvalues of H_n, are distributed when $n \to \infty$. The solution is easily obtained. From (2.18) the zeros of $P_n(x; E)$ in the band are given by

$$\Theta_{n+1}(x; E) = j\pi \qquad j = 1, 2, 3, \ldots, n.$$

Hence the integrated distribution function of the zeros are expressed in E^- as

$$\nu_n(x; E) = 1 - \frac{1}{n}\operatorname{int}\left(\frac{1}{\pi}\Theta_{n+1}(x; E)\right). \tag{5.2}$$

Here E^- is the set such that the points of the band edges are removed from E, int[·] denotes the integral part, and $\nu_n(x; E)$ is normalised as $\nu_n(B_m+0; E)=0$ and $\nu_n(A_1-0; E)=1$. By virtue of theorem 3 the limit function of $\nu_n(x; E)$ exists and is given by

$$\nu(x; E)=1-(1/\pi)\arg\Phi(x+\mathrm{i}0; E) \tag{5.3}$$

which is called the equilibrium distribution (Hille 1962) and is equal to the charge distribution function in the system of conductors considered in § 3. The resultant limit expression is written by the EMF only, and so is independent of the band shape, although $\nu_n(x; E)$ for small n is no doubt affected by the band shape.

The asymptotic (differential) distribution function of the zeros is thus given by

$$\frac{\mathrm{d}}{\mathrm{d}x}\nu(x; E)=-\frac{1}{\pi}\frac{\mathrm{d}}{\mathrm{d}x}\left(\arg\Phi(x+\mathrm{i}0; E)\right)=\begin{cases}(1/\pi)|X(x; E)| & x\in E^-\\ 0 & \text{otherwise.}\end{cases} \tag{5.4}$$

From the explicit form (4.9) of $X(x; E)$ we can say that the eigenvalues of the truncated Hamiltonian matrix are distributed nearly uniformly except near the band edges where the distribution function diverges by the $-\frac{1}{2}$th power.

When the recursion method is used, the eigenvalues of H_n are sometimes discussed in order to examine the band shape, but the present result indicates that such an attempt is absurd, at least for large n.

If we denote the zeros of $P_n(x; E)$ by x_{ni} $(i=1, 2, \ldots, n)$, then we have

$$\sum_{i=1}^{n} x_{ni}=\sum_{j=0}^{n-1} a_j \qquad \sum_{i=1}^{n} x_{ni}^2=\sum_{j=0}^{n-1} a_j^2+2\sum_{j=0}^{n-2} b_j^2 \tag{5.5}$$

which are obtained by calculating the traces of H_n and H_n^2, respectively. Using (5.4) we can calculate the limit of $1/n$ times the left-hand sides of (5.5). For example the first equation of (5.5) is reduced to

$$\int_E x\,\mathrm{d}\nu(x; E)=\lim_{n\to\infty}\left(\frac{1}{n}\sum_{j=0}^{n-1} a_j\right).$$

The integral in the left-hand side can be evaluated by the contour integral, where the residue at infinity is used, and the resultant relation coincides with the first one in (4.26). If the second equation of (5.5) is dealt with, we again have the second one in (4.26). The third and succeeding relations in (4.26) can also be obtained by calculating the traces of H_n^3 and higher powers.

The other problem concerns how much the truncated basis W_n contains the state with eigenenergy x. For this purpose the quantity

$$\Omega_n(x; E)=\frac{1}{n}\sum_{j=0}^{n-1}|\langle x|j\rangle|^2=\frac{1}{n}|\langle x|0\rangle|^2\sum_{j=0}^{n-1}[p_n(x; E)]^2 \tag{5.6}$$

is examined as a function of x.

As mentioned in § 2, the expression (2.18) of $P_n(x; E)$, which we intend to use, is not valid at the band edges or at the singularities of $G(z; E)$. In the following arguments we use it without making reference to these singularities. Note therefore that these points are implicitly excluded and that the results are not necessarily valid throughout the band.

We refer to the famous Christoffel-Darboux formula

$$\sum_{j=0}^{n-1}(p_j(x; E))^2=b_{n-1}(p_{n-1}(x; E)p_n'(x; E)-p_n(x; E)p_{n-1}'(x; E))$$

and use the expression (2.18) of $P_n(x; E)$. Then we have

$$\pi w(x)\frac{1}{n}\sum_{j=0}^{n-1}(p_j(x; E))^2$$
$$= -\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{1}{n}\Theta_n(x; E)\right) + \frac{1}{\sin\theta_n(x; E)}\mathrm{o}(n) \qquad \mathrm{o}(n)\to 0 \text{ as } n\to\infty.$$

The second term in the right-hand side vanishes as $n\to\infty$, if $\sin\theta_n(x; E)$ has a positive lower bound, which is the case except for the band edges or the points where $w(x)=0$. Hence we have

$$\pi w(x)\lim_{n\to\infty}\frac{1}{n}\sum_{j=0}^{n-1}[p_j(x; E)]^2 = |X(x; E)| \qquad \text{for } w(x)>0$$

and it follows that

$$\lim_{n\to\infty}\Omega_n(x; E) = \frac{1}{\pi N(x)}|X(x; E)| \qquad \text{for } N(x)>0 \text{ and } |\langle x|0\rangle|\neq 0. \tag{5.7}$$

This result is somewhat surprising. The asymptotic form of $\Omega_n(x)$ is independent of the initial state $|0\rangle$, except for some energy eigenstates $|x\rangle$ to which the state $|0\rangle$ is accidentally orthogonal.

6. Simple cases

As is seen in § 4, the EMF is written by use of hyperelliptic integrals (see appendix 2 for the two-band case), and thus the numerical integration is inevitable in general. In several cases, however, some results can be obtained elementarily and are given in the following subsections.

6.1. Single-band

This case is elementary. For simplicity we let $E=[-1, 1]$, then there is no saddle point and thus $\mathrm{d}\phi(z; E)/\mathrm{d}z = -1/(z^2-1)^{1/2}$, from which we have the famous Joukowski transformation as the EMF

$$\Phi(z; E) = \tfrac{1}{2}[z+(z^2-1)^{1/2}] \tag{6.1}$$

and $\gamma(E)=\frac{1}{2}$. This EMF has already appeared in the Szegö theory. We may obtain

$$\lambda_1 = 0 \qquad \lambda_2 = \tfrac{1}{2} \qquad \lambda_3 = 0 \qquad \lambda_4 = \tfrac{3}{8} \qquad \ldots.$$

These values suggest the convergence of the recursion coefficients (see (4.17) and (4.26)).

6.2. Symmetric two bands

Here we mean the symmetric support, and the symmetric band shape is not assumed. Suppose for simplicity $E=[-A, -B]+[B, A]$, then one saddle point exists, which is evidently located at zero. Thus the EMF and other characteristic quantities are written as

$$\Phi(z; E) = \tfrac{1}{2}[(z^2-A^2)^{1/2}+(z^2-B^2)^{1/2}] \tag{6.2}$$
$$\gamma(E) = \tfrac{1}{2}(A^2-B^2)^{1/2} \qquad q_1 = q_2 = \pi$$
$$\lambda_1 = 0 \qquad \lambda_2 = \tfrac{1}{2}(A^2+B^2) \qquad \lambda_3 = 0 \qquad \lambda_4 = \tfrac{1}{8}(3A^4+2A^2B^2+3B^4), \ldots. \tag{6.3}$$

Hence the asymptotic oscillations of the recursion coefficients are of double period. Let the asymptotic doubles be

$$(a_0, b_0), (a_1, b_1), (a_0, b_0), (a_1, b_1), \ldots$$

then from (4.26), (4.27) and (6.3)

$$a_0 + a_1 = 0 \qquad b_0, b_1 = \tfrac{1}{2}[(A^2 - a_0^2)^{1/2} \pm (B^2 - a_0^2)^{1/2}].$$

This result says that when E is fixed the asymptotic oscillations are characterised only by a single parameter, say a_0, which depends on the band shape.

6.3. Integral periods

The case where the recursion coefficients have integral period was investigated by TDT. In the present theory this means that charges on all component continua are given by integral multiples of $2\pi/p$, p being a period (integer).

Consider the conformal mapping from z plane to ζ plane given by

$$\Pi_p(z) = \zeta^p + c^2/\zeta^p \tag{6.4}$$

where all coefficients of $\Pi_p(x)$ are real and c is a positive constant. Suppose that $\Pi_p(z)$ and c are so chosen that each of the following two algebraic equations

$$\Pi_p(z) = \pm 2c \tag{6.5}$$

has p real roots, where multiple roots are also allowed. Thus all roots of $\mathrm{d}\Pi_p(x)/\mathrm{d}x = 0$ are real. Let

$$E = \{x \mid -2c \leqslant \Pi_p(x) \leqslant 2c\}$$

then E is a union of at most p disjoint line segments, but here it is regarded as a union of p segments, some of which are joined with each other when multiple roots exist. From (6.4) we have

$$-\frac{\mathrm{d}}{\mathrm{d}z}[\ln \zeta] = -\frac{1}{p} \frac{\mathrm{d}\Pi_p(z)/\mathrm{d}z}{(\Pi_p(z)^2 - 4c^2)^{1/2}} \tag{6.6}$$

which denotes that the present mapping is the EMF such that $E \to \gamma(E) = c^{1/p}$. The band edges and the saddle points are given by the roots of (6.5) and the extrema of $\Pi_p(x)$, respectively, some of which are degenerate in the multiple-root case. The charge in each segment can be calculated by an elementary integration (see (4.13)) and is equal to $2\pi/p$, which meets our requirement. When $p = 2$, we have the same result as in the preceding symmetric two-band case.

The present result coincides with that obtained by TDT who investigated a periodic linear chain by the Bloch theorem.

7. Conclusions

In this paper the recursion method is investigated analytically with main attention on its asymptotic properties in the multiband (band gap) case. The correspondence between the support of the spectrum and the asymptotic behaviours of the recursion coefficients is clarified.

When the band satisfies the Geronimus condition, then the limit relations of the recursion coefficients such as (4.17) and (4.26) are derived through the EMF. Only the support E of the band is made use of, and thus they contain E (i.e. the positions of the band edges) as a parameter, and are independent of the band shape. The characteristic quantities in the present theory are as follows, each of which is a function of E only.

(i) Saddle points s_k ($k=1, 2, \ldots, m-1$), which are needed to calculate succeeding characteristic quantities.

(ii) Transfinite diameter $\gamma(E)$, which is equal to the limit of the geometric mean of b_n.

(iii) Charges q_k ($k=1, 2, \ldots, m$) on the component line segments, which are related to the period of the asymptotic oscillations.

(iv) λ_i ($i=1, 2, 3, \ldots$), which correspond to the limits of the arithmetic means of the terms including the powers of a_n and b_n. The arithmetic mean of a_n converges to λ_1.

When the asymptotic properties of the truncated basis are examined, the function $X(x; E)$ defined by (4.9) plays an important role, and it also depends on E only.

Our consequences are no doubt in accord with the TDT numerical results, as is discussed in § 4.5. In order to make more detailed numerical examination concerning such as the higher-order terms in (4.26) and the results in § 5, we have also carried out the numerical experiments and the results will be reported in the near future.

The present problem can be interpreted in a different manner. We have considered how the asymptotic recursion coefficients are restricted by the spectrum of the band. This is the inverse problem of a discrete Hill equation and is related to the periodic wave solution in the Toda lattice with exponential interactions (see Toda 1981). The limit relations (4.26) correspond to the conservation ones in this lattice.

Appendix 1. Transfinite diameter and Tchebycheff constant

In this appendix the definitions of the transfinite diameter and the Tchebycheff constant as functions of a closed set E are given without proof. For the proofs and the details see Tsuji (1959, p 53) or Hille (1962, p 264).

The transfinite diameter is originally defined as follows. Let $t_n(E)$ be the $[\frac{1}{2}n(n-1)]$th root of the maximum among the absolute values of the Vandermonde determinants over n variables on E, i.e.

$$[t_n(E)]^{n(n-1)/2} = \max_{z_{n1}, z_{n2}, \ldots \in E} \prod_{1 \leqslant i \leqslant j \leqslant n} |z_{ni} - z_{nj}|.$$

Then the sequence $\{t_n(E)\}$ is obviously non-negative and can be proved to be monotone non-increasing. Therefore the limit of $t_n(E)$, say $\tau(E)$, exists, which is the transfinite diameter of E.

The Tchebycheff constant, say $\rho(E)$, is defined as the limit of the nth root of the maximum absolute value of the Tchebycheff polynomial of degree n defined on E, i.e.

$$\rho(E) = \lim_{n\to\infty} (M(T_n(\cdot\,; E); E))^{1/n}.$$

The equalities $\tau(E) = \rho(E) = \gamma(E)$ are well known in the analytic potential theory, $\gamma(E)$ being the logarithmic capacity.

Appendix 2. Expressions by elliptic functions in the two-band case

In the two-band case ordinary elliptic integrals appear, and thus the characteristic quantities can be written by use of the (Jacobi) elliptic functions. It requires some tedious calculation to obtain the simplified expressions and here we give them without derivation.

We let

$$w_1 = A_1 - B_1 \qquad w_2 = A_2 - B_2 \qquad g = B_1 - A_2$$

and do not write the symbol E as the support since it is customarily used as the complete elliptic integral. The modulus of the elliptic functions given by

$$k^2 = g(w_1 + w_2 + g)/[(w_1 + g)(w_2 + g)]$$

is common to the following expressions. The results are

$$\gamma = \tfrac{1}{4}(w_1 + w_2)(1 - k^2)^{-1/4} \exp\left(- \int_0^u Z(u)\,\mathrm{d}u \right)$$

$$q_1/\pi = 1 + u/K \qquad q_2/\pi = 1 - u/K$$

$$s_1 = \tfrac{1}{2}\{(B_1 + A_2) - g \operatorname{sn} u + [(w_1 + g)(w_2 + g)]^{1/2} Z(u)\}$$

where u is defined by $\operatorname{sn} u = (w_1 - w_2)/(w_1 + w_2)$ and the Jacobi zeta function is used:

$$u = \int_0^{\operatorname{sn} u} (1 - k^2 t^2)^{-1/2}(1 - t^2)^{-1/2}\,\mathrm{d}t$$

$$Z(u) = \int_0^{\operatorname{sn} u} (1 - k^2 t^2)^{1/2}(1 - t^2)^{-1/2}\,\mathrm{d}t - (E/K)u$$

K and E being the complete elliptic integrals of the first and the second kinds respectively.

For the numerical evaluation these expressions seem to be less useful, if the computer is available, than the numerical integration of $X(x; E)$ by which the estimates in § 4.5 are obtained.

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