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Analytic expressions for asymptotic forms of continued-fraction coefficients in the presence of a spectral gap

Sayaka Yoshino

Institute of Materials Science, University of Tsukuba, Tsukuba, Ibaraki 305, Japan

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Abstract. It is shown that the recursion method, i.e. the continued-fraction expansion of the diagonal element of the resolvent, is equivalent to the exponential Toda lattice in the sense that the limiting identities in the former method have the same forms as the conservation laws in the latter lattice. The asymptotic continued-fraction coefficients (recursion coefficients) are then related to a particular motion in the Toda lattice. As a result of this relation, the analytic expressions for the simply oscillating asymptotic recursion coefficients in the two-band (single-gap) case are given explicitly in terms of the Jacobian elliptic functions and in the Fourier series forms.

1. Introduction

The recursion method in condensed matter physics (Haydock 1980, Pettifor and Weaire 1985) is known as a powerful and lucid approximation as far as the case with a single-band spectrum is treated. This method is nothing but the evaluation of the diagonal element of the resolvent by use of the infinite continued Jacobi-fraction (J-fraction). Here the coefficients of the J-fraction, which are referred to as recursion coefficients, are computed from the Hamiltonian and the state with respect to which the diagonal element is taken.

The success of the recursion method in the single-band case is largely due to the convergence of the recursion coefficients, i.e. to the utility of the traditional constant termination (replacement of the recursion coefficients beyond an adequate stage by their limits). On the contrary, if spectral gaps exist (multiband case), i.e. if the support of the spectrum is composed of two or more segments, then they do not converge and they exhibit asymptotically oscillating behaviours. Numerical experiments (Turchi *et al* 1982, Haydock and Nex 1985, Anlage and Smith 1986) suggest that their asymptotic behaviours are well ordered and thus there may exist simple analytic expressions for their asymptotic forms.

In a preceding paper (Yoshino 1987, hereafter referred to as I) the present author developed an analytic theory to investigate the asymptotic properties of the recursion method applicable to the multiband case. In I various asymptotic (limiting) relations of the recursion coefficients were derived, and the period of their asymptotic oscillations was written as a function of the support of the spectral function. Analytic expressions for their asymptotic forms, however, were not given. The purpose of this paper is to ascertain them in the two-band case. We have two reasons to treat this simple case: one is that this case seems to be much more important for practical applications and the other is that rather familiar functions (the Jacobian elliptic and the theta functions) are available.

This paper is outlined as follows. First in § 2 we give the analytic results that are obtained in I and are needed for the arguments in this paper. The numerical examples in § 3 suggest that the asymptotic recursion coefficients in the two-band case are simply periodic and are expanded in the Fourier series where the constant and the principal terms are dominant. In § 4, which is the main part of this paper, we point out that the limiting relations obtained in I have the same forms as the conservation laws in the Toda lattice with exponential interactions (Toda 1967, 1981). The recursion coefficients correspond to the Lax-pair variables (at a certain instant) in the Toda lattice, if the order of the former coefficients is regarded as the mass index in the latter lattice. This connection enables us to express the asymptotic forms of the recursion coefficients by use of the periodic solution in the Toda lattice. The explicit expressions in the two-band case are then given. In § 5 we give some remarks as concerns our results, and finally in § 6 this paper is summarised.

2. Survey of the analytic results

Our problem is as follows. Suppose that the diagonal element of the resolvent, which is equal to the Stieltjes transform of an adequate spectral function, is written in the form of the infinite continued J-fraction

$$\begin{aligned}\langle 0|(z-H)^{-1}|0\rangle &= \int_E (z-x)^{-1}\,\mathrm{d}\mu(x)\\ &= 1/\{z-a_0-b_0^2/[z-a_1-b_1^2/(z-a_2-b_2^2/\ldots)]\}.\end{aligned} \tag{1}$$

Here H is the Hamiltonian under consideration and the state $|0\rangle$ is assumed to be normalised. The spectral function, which we refer to as the band, is denoted by $\mathrm{d}\mu(x)=w(x)\,\mathrm{d}x$, and E is its support. The pairs of coefficients $\{a_n, b_n\}$ (both real and $b_n>0$, $n=0,1,2,\ldots$) are the recursion coefficients. Then how are their asymptotic forms expressed?

In the recursion method a_n and b_n are calculated successively from H and $|0\rangle$, accompanied with the generation of the semi-infinite sequence of states (kets) orthonormal to each other. The semi-infinite-dimensional matrix representative of H by using this sequence as a basis is real-symmetric and tridiagonal, and its diagonal and subdiagonal elements are given by the a_n and b_n respectively:

$$H=\begin{pmatrix} a_0 & b_0 & & \\ b_0 & a_1 & b_1 & \\ & b_1 & a_2 & b_2 \\ & & \ddots & \ddots & \ddots \end{pmatrix}. \tag{2}$$

In the following our analytic results are briefly presented (for details see I). Although we are concerned with the single-gap case in this paper, we here refer to the general multigap case since the multigap description seems to be more transparent. The band is thus assumed to be composed of m subbands, and its support is written as $E=[B_m, A_m]+\ldots+[B_2, A_2]+[B_1, A_1]$, where A_k and B_k ($k=1,2,\ldots,m$) are given in descending order.

We now consider the following electrostatic problem. We regard E as the union of m segment conductors arranged in a two-dimensional complex plane, and assume that the continuous electric charge 2π is distributed on E such that all potentials of

m components are kept to be equal to one another. We then define the complex potential $\phi(z)$, which behaves at infinity as $-\ln z+O(1/z)$.

The relevant characteristic quantities are as follows.

(i) There exist $m-1$ saddle points of the electrostatic potential. They are denoted by s_k $(k=1,2,\ldots,m-1)$.

(ii) The transfinite diameter of E denoted by γ. The electrostatic potential of the conductors is given by $\ln(1/\gamma)$.

(iii) The individual electric charges distributed on the conductors. We denote them as q_k on the kth component $[B_k, A_k]$ $(k=1,2,\ldots,m)$.

(iv) The coefficients in the Taylor series (at infinity) of $\mathrm{d}\phi(z)/\mathrm{d}z$. We define λ_r $(r=1,2,3,\ldots)$ by

$$-\frac{\mathrm{d}\phi(z)}{\mathrm{d}z}=\frac{1}{z}+\sum_{r=1}^{\infty}\frac{\lambda_r}{z^{r+1}}. \tag{3}$$

For $r=1,2$ we have

$$\lambda_1=\tfrac{1}{2}\sum_{k=1}^{m}(A_k+B_k)-\sum_{k=1}^{m-1}s_k \tag{4a}$$

$$\lambda_2=\tfrac{1}{4}\sum_{k=1}^{m}(A_k^2+B_k^2)-\tfrac{1}{2}\sum_{k=1}^{m-1}s_k^2+\tfrac{1}{2}\lambda_1^2. \tag{4b}$$

Note that all the characteristic quantities are functions of the support E (i.e. A_k and B_k $(k=1,2,\ldots,m)$) and only of E, i.e. they do not depend on the *band shape*. Here we use this term, as in I, to make reference to the variety of spectral functions with the same support.

We assume that $\mu(x)$ satisfies the Geronimus condition

$$\lim_{\delta\to+0}\delta^{1/2}\ln a(\delta)=0 \qquad a(\delta)=\inf_{[x,x+\delta]\subset E}[\mu(x+\delta)-\mu(x)]$$

which is a sufficient condition for the analytic properties given below. We see that this condition, which restricts the rate of the decrease of $w(x)$ when it drops to zero, is satisfied by ordinary spectra (e.g. a spectrum with power-law decrease), except for the one with very singular tails such as $\mu(x)-\mu(0)\sim\exp(-1/x^c)$ $(c\geqslant\frac{1}{2})$ at $x\to+0$. In this paper we hereafter assume that this condition is satisfied.

In I various asymptotic (limiting) properties have been obtained analytically and are as follows.

(i) The transfinite diameter equals the limit of the geometric mean of b_n

$$\lim_{n\to\infty}\left(\prod_{j=0}^{n-1}b_j\right)^{1/n}=\gamma. \tag{5}$$

(ii) As concerns the arithmetic means of the products of a_n and b_n, we have the following limiting relation:

$$\lim_{n\to\infty}\frac{1}{n}\operatorname{Tr}[H_n^r]=\lambda_r \qquad r=1,2,3,\ldots. \tag{6}$$

Here H_n is the n-dimensional matrix obtained by truncating H (see equation (2)). It is obvious that the left-hand side of equation (6) is written by the limiting arithmetic mean of the sum of rth-degree products of a_n and b_n. In particular for $r=1,2$ we may write

$$\lim_{n\to\infty}\frac{1}{n}\sum_{j=0}^{n-1} a_j=\lambda_1 \tag{6a}$$

$$\lim_{n\to\infty}\frac{1}{n}\sum_{j=0}^{n-1} (a_j^2+2b_j^2)=\lambda_2. \tag{6b}$$

(iii) The period of the asymptotic oscillations of a_n and b_n is determined by q_k in such a manner as their asymptotic forms may be written as $F(nq_1, nq_2, \ldots, nq_{m-1})$, where $F(\ldots)$ stands for a periodic function with period 2π with respect to all arguments.

3. Numerical examples

In this section the asymptotic forms of the recursion coefficients are speculated from the numerical tests given below. Our tests are simple. We treat two kinds of supports, say E_1 and E_2, and two kinds of band shapes for each support. Table 1 gives the positions of the band edges of these supports and also the values of the characteristic quantities calculated numerically. The figures in the period column bear the same meaning as in I, i.e. the asymptotic recursion coefficients for the support E_1 (E_2) will look like a mixture of two (three) subsequences with period 20.5 (78.3).

Table 1. The characteristic quantities of the supports treated in this paper.

E	Band edges	s_1	λ_1	γ	$\ln\gamma$	$q_1/2\pi$	Period
E_1	[0,1.5]+[2.5,3.5]	2.011 27	1.738 73	0.837 67	−0.177 13	0.451 26	2-20.5
E_2	[0,2]+[3,3.5]	2.542 47	1.707 53	0.828 71	−0.187 88	0.346 06	3-78.3

The first 60 pairs, $\{a_n, b_n\}$ ($n=0,1,2,\ldots,59$), are computed in each case and are shown in figure 1. Remembering that the geometric mean converges as concerns b_n, we plot $\ln b_n$ instead of b_n itself. We see that in every case the asymptotic behaviour appears only after several recursion steps. It is readily seen from figure 1 that the arithmetic means of a_n and $\ln b_n$ are nearly equal to λ_1 and $\ln\gamma$, respectively (see equations (6a) and (5)). We do not give here a more quantitative analysis or estimates of higher-degree relations in equation (6).

We examine the period of the asymptotic oscillations. As mentioned in § 2 the asymptotic forms of a_n and b_n should be written by periodic functions of period 2π with argument nq_1. In figure 2 the plots of $\cos(nq_1)$ and $\cos[(n+\frac{1}{2})q_1]$ as functions of n are given as typical examples of such periodic functions. Note that the phase difference between two plots is $\frac{1}{2}q_1$. Comparing figures 1 and 2 we see that the asymptotic oscillating deviations of a_n and $\ln b_n$ from their arithmetic means may be well approximated by single sinusoidal functions. In addition the phase of the oscillations of $\ln b_n$ seems to differ by nearly $\frac{1}{2}q_1$ from that of a_n irrespective of the band shape. That is to say, we have for $n\gg 1$

$$a_n-\lambda_1\sim C^a\cos(nq_1+\alpha) \qquad C^a>0$$

$$\ln(b_n/\gamma)\sim C^b\cos[(n+\tfrac{1}{2})q_1+\alpha] \qquad C^b>0$$

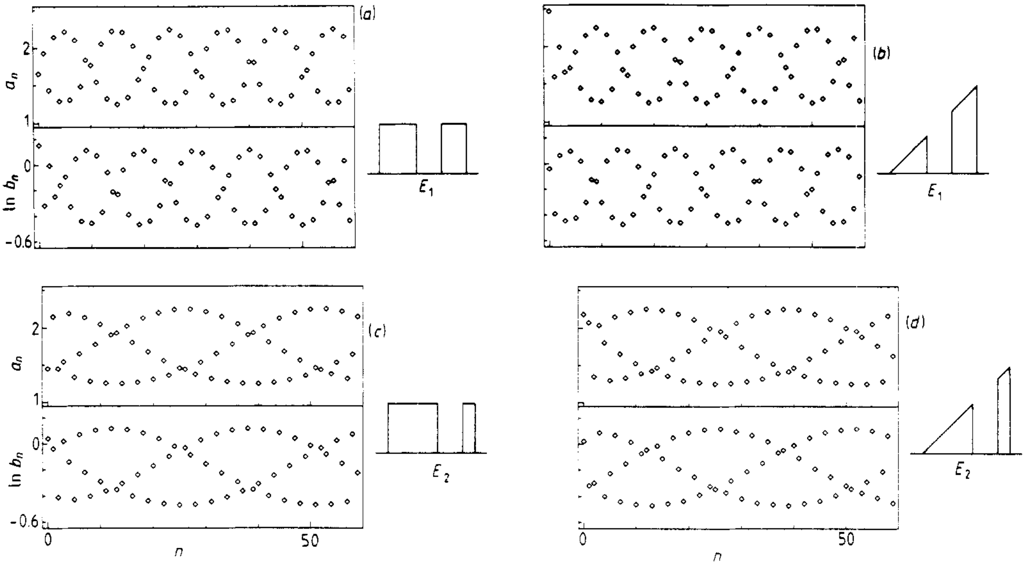

Figure 1. Computed recursion coefficients. The band shape is shown at the right of each plot. The support is E_1 in (a) and (b) and E_2 in (c) and (d).

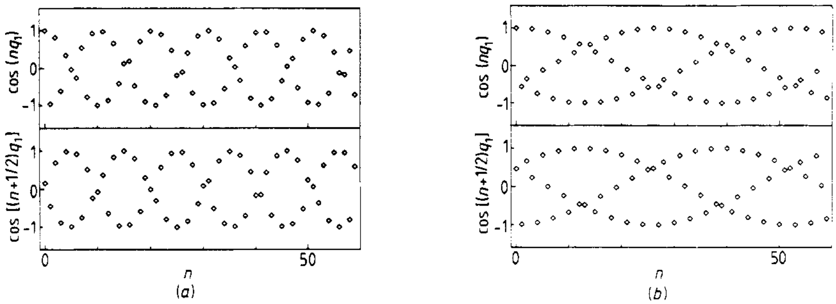

Figure 2. Plots of sinusoidal functions with the period asserted by our theory. The periods in (a) and (b) are those peculiar to the supports E_1 and E_2, respectively. Thus (a) corresponds to figures 1(a) and 1(b) and (b) corresponds to figures 1(c) and 1(d).

if we choose a phase constant α adequately. As was pointed out by Turchi *et al* (1982), both the C^a and C^b seem to be independent of the band shape. On the contrary the phase constant α may depend on it. Haydock and Nex (1985) claimed that α depends on the ratio of the spectral weights of two subbands (integrals of $w(x)$ over individual subbands).

Now we may claim the following as concerns the effect of $w(x)$ on the asymptotic forms of the recursion coefficients. The asymptotic forms depend on $w(x)$ through two parameters: one is the support E and the other is the above-mentioned phase constant α. It is α that depends on the band shape. The asymptotic recursion coefficients are written as

$$\begin{aligned} a_n &= F^a(nq_1+\alpha;\, E) \\ \ln b_n &= F^b((n+\tfrac{1}{2})q_1+\alpha;\, E) \end{aligned} \tag{7}$$

where both the $F^a(.; E)$ and $F^b(.; E)$ are periodic with period 2π with respect to the first arguments. Suppose that their Fourier expansions are given by

$$\begin{aligned} F^a(x; E) &= C_0^a + C_1^a \cos x + \sum_{j=2}^{\infty} (C_j^a \cos jx + S_j^a \sin jx) \\ F^b(x; E) &= C_0^b + C_1^b \cos x + \sum_{j=2}^{\infty} (C_j^b \cos jx + S_j^b \sin jx). \end{aligned} \tag{8}$$

Note that the phase constant α has been so chosen that the terms containing $\sin x$ do not appear. Then $C_0^a(=\lambda_1)$ and $C_0^b(=\ln \gamma)$ are already ascertained, $C_1^a(>0)$ and $C_1^b(>0)$ depend on E only, and in each of the expansions (8) the first two terms are dominant. As will be shown in § 4.4, S_j^a and S_j^b vanish also for $j \geqslant 2$.

4. Analytic expressions via the Toda lattice

In this section we intend to express analytically the asymptotic forms of the recursion coefficients in the two-band case. They should be simply periodic (with respect to n) and should satisfy the limiting properties given in § 2.

4.1. *The C-free condition*

First we emphasise that an analytic expression, if it exists, is restricted severely in its form by the limiting relations (5) and (6). We put forth the following arguments. We may assume the asymptotic form (7). For example, we consider the relation (6a). Suppose that $q_1/2\pi$ is rational with p being the denominator of its irreducible fraction, then the left-hand side of equation (6a) can be replaced by the sum

$$(1/p) \sum_{j=0}^{p-1} F^a((2\pi/p)j + \alpha; E). \tag{9a}$$

If $q_1/2\pi$ is irrational, on the other hand, it is evidently replaced by the integral

$$(1/2\pi) \int_0^{2\pi} F^a(x; E)\, \mathrm{d}x. \tag{9b}$$

We know that q_1 can be varied arbitrarily, continuously and thus infinitesimally. We may therefore claim that the analytic expression $F^a(nq_1 + \alpha; E)$, which is to vary continuously as q_1, must have such a property that the sum (9a) assumes the same value as the integral (9b), since for an arbitrary rational case of $q_1/2\pi$ there exists an irrational case in its arbitrary neighbourhood. In other words, we may state that it must make no alteration on the analytic form whether we consider a commensurate or an incommensurate case. This condition will be referred to as the C-free (commensurability-free) condition. Here we should observe the dependence of $F^a(.; E)$ on the second argument E, which cannot be invariant when q_1 varies even though the variation is infinitesimal. Strictly speaking, it is this dependence that is restricted by the present argument (see appendix 1).

The C-free condition is imposed on every higher-degree term in equation (6) and also on the logarithmic version of equation (5). It thus seems to be practically impossible to ascertain such an analytic form that satisfies the C-free condition completely. We are, however, fortunate enough to know the system that bears the identities of the same forms as equations (5) and (6) and hence satisfies the C-free condition. It is the Toda lattice (Toda 1967, 1981) and in the subsequent subsections we will make use of the solutions of this lattice.

4.2. *The Toda lattice in the Lax form*

We write the equation of motion for the classical non-linear lattice dynamics in the infinite (not semi-infinite) Toda lattice as

$$\frac{d^2}{dt^2} Q_n = \exp(Q_{n-1} - Q_n) - \exp(Q_n - Q_{n+1}) \tag{10}$$

where $Q_n \equiv Q_n(t)$ (t is time) is the displacement of the nth mass ($-\infty < n < \infty$). The infinite lattice is necessary since we intend to observe not only commensurately but also incommensurately periodic waves. The equation of motion (10) has the following property. If $Q_n(t)$ is a solution of equation (10), then

$$\tilde{Q}_n(t) = Vt + Cn + C' + Q_n(t\,e^{-C/2}) \tag{11}$$

is also a solution with V, C and C' being arbitrary constants.

Let us analyse equation (10) according to the Lax-form treatment of Flaschka (1974). Let

$$\begin{aligned} a_n(t) &= \frac{d}{dt} Q_n(t) \\ b_n(t) &= \exp[\tfrac{1}{2}(Q_n(t) - Q_{n+1}(t))] \end{aligned} \tag{12}$$

and $L(t)$ be the infinite-dimensional real-symmetric and tridiagonal matrix, whose diagonal elements (n, n) and subdiagonal elements $(n, n+1)$ or $(n+1, n)$ are the $a_n(t)$ and $b_n(t)$ respectively. The semi-infinite-dimensional version of $L(t)$ has the same form as H (see equation (2)). Then it can be proved that $L(t)$ is orthogonally similar to $L(0)$, i.e. the eigenvalues of $L(t)$ are independent of t. Here we have used slightly different notations from those by Flaschka, i.e. the roles of $a_n(t)$ and $b_n(t)$ are here exchanged for each other, and Flaschka multiplied the right-hand sides of equations (12) by $\pm\frac{1}{2}$. The former is in order to make clear the equivalence to the recursion method, and the latter modification is not substantial for the Lax-form treatment.

Now we may obtain a set of conservation laws, which states that the trace of every power of $L(t)$ is a constant of motion. Since we are treating the infinite lattice, it should be written as

$$\lim_{n\to\infty} \frac{1}{n} \mathrm{Tr}[L_n(t)^r] = \text{independent of } t \qquad r = 1, 2, 3, \ldots \tag{13}$$

where $L_n(t)$ is the truncated n-dimensional version of $L(t)$ whose entry runs from 0 to $n-1$. Equation (13) evidently has the same form as equation (6), the right-hand side of which should be read as being independent of α, the band-shape parameter. It is obvious that this set of conservation laws is free from the commensurability. Hence, if we find a solution in the Toda lattice such that $a_n(t)$ and $b_n(t)$ are simply periodic, then we may use this solution as an analytic expression for the asymptotic recursion coefficients in the two-band case.

4.3. A simply periodic motion in the Toda lattice

In this and subsequent subsections we use the elliptic theta functions and the Jacobian elliptic functions. Our notation of the theta functions agrees with that of Erdélyi (1953), i.e. they are denoted by $\theta_j(v, q)$ ($j = 1, 2, 3, 4$) with the period of θ_1 and θ_2 being two and that of θ_3 and θ_4 being unity. The second argument of the theta functions is here called a nome and is not explicitly written for simplicity. As concerns the Jacobian functions, e.g. $\mathrm{sn}(u, k)$, we also omit the modulus k, which has the well known one-to-one correspondence to the nome. According to the convention the symbol K denotes the real quarter-period of $\mathrm{sn}(u, k)$. Hereafter we always use the symbols q and k to denote the nome and the modulus, respectively. We note that the q_1 and q_2 defined in § 2 to denote the distributed charges should be distinguished from the nome q.

A simply periodic motion in the Toda lattice was obtained by Toda (1967). Properly speaking, Toda constructed this lattice from the requirement for a wave-like motion. We are concerned with a solution such that $a_n(t)$ and $b_n(t)$ (not necessarily $Q_n(t)$) are simply periodic with respect to n. The solution with wavenumber κ and frequency ω is written as

$$Q_n(t) = Vt + Cn + C' + \ln[\theta_4(v_{n-1})/\theta_4(v_n)] \tag{14}$$

$$v_n \equiv v_n(t) = (\kappa n - \omega t + \delta)/2\pi \tag{15}$$

where V, C, C' and δ are arbitrary. We observe that $a_n(t)$ and $b_n(t)$ are always periodic irrespective of C, although $Q_n(t)$ is not periodic when $C \neq 0$. Equation (11) implies that when C is varied then the timescale must be altered simultaneously according to C. We, however, need not alter explicitly the timescale. This is because the solution (14) depends on t through the form of ωt, which can be left unaltered if ω is redefined adequately (the dependence through Vt is not significant since V is arbitrary). The dispersion relation expressing ω as a function of κ thus contains C, and is written as†

$$\omega/2\pi = \pm \mathrm{e}^{-C/2}\theta_1(\kappa/2\pi)/\theta_1'(0). \tag{16}$$

Relation (16) is easily obtained by substituting equation (14) into equation (10) and using the following identities of the theta functions:

$$\frac{\mathrm{d}^2}{\mathrm{d}v^2}\ln\theta_4(v) = \left(\frac{\theta_1'(0)}{\theta_2(0)}\right)^2\left(\frac{\theta_3(v)}{\theta_4(v)}\right)^2 - 4KE$$

$$\theta_4(v+w)\theta_4(v-w)\theta_2^2(0) = \theta_4^2(v)\theta_2^2(w) + \theta_3^2(v)\theta_1^2(w).$$

The first identity, where the symbol E is used to denote the complete elliptic integral of the second kind, is obtained by taking the derivative of the Jacobian zeta function: $\mathrm{Z}(u) = (\mathrm{d}/\mathrm{d}u)\ln\theta_4(u/2K)$. The latter identity is the addition formula (see Whittaker and Watson 1927). Note that the nome q (or the corresponding modulus k) is arbitrary but is common to both equations (14) and (16).

From equations (12) and (14) we obtain

$$\begin{aligned} a_n(t) &= V + \left(\frac{\omega}{2\pi}\right)\left(\frac{\theta_4'(v_n)}{\theta_4(v_n)} - \frac{\theta_4'(v_{n-1})}{\theta_4(v_{n-1})}\right) \\ b_n(t) &= \mathrm{e}^{-C/2}\frac{[\theta_4(v_{n-1})\theta_4(v_{n+1})]^{1/2}}{\theta_4(v_n)}. \end{aligned} \tag{17}$$

† This dispersion relation is different from that by Toda (1981, equation (2.3.2)). It seems that Toda was misled.

In equations (14) and (17) we can replace all $\theta_4(v)$ simultaneously by $\theta_3(v)$, since $\theta_3(v+\frac{1}{2})=\theta_4(v)$ and δ in equation (15) is arbitrary.

We now refer to the Fourier expansions (q expansions) of $\ln[\theta_4(v)/\theta_4(0)]$ and $\theta_4'(v)/\theta_4(v)$ (Erdélyi 1953, p 358). The expansions of $a_n(t)$ and $\ln b_n(t)$ are then written as (leading terms only)

$$\begin{aligned} a_n(t) &= V+4\omega q(1-q^2)^{-1}\sin(\tfrac{1}{2}\kappa)\cos[\kappa(n-\tfrac{1}{2})-\omega t+\delta]+\ldots \\ \ln b_n(t) &= -\tfrac{1}{2}C+4q(1-q^2)^{-1}\sin^2(\tfrac{1}{2}\kappa)\cos(\kappa n-\omega t+\delta)+\ldots \end{aligned} \tag{18}$$

from which it follows that

$$\lim_{n\to\infty}\frac{1}{n}\sum_{j=0}^{n-1}a_j(t)=V \tag{19a}$$

$$\lim_{n\to\infty}\left(\prod_{j=0}^{n-1}b_j(t)\right)^{1/n}=\mathrm{e}^{-C/2}. \tag{19b}$$

Equations (19a) and (19b) correspond to the limiting relations (6a) and (5) in the recursion method, respectively.

4.4. *Analytic expressions for the asymptotic recursion coefficients*

Now we may use equations (17) as the analytic expressions for the asymptotic recursion coefficients in the two-band case. Equations (17) and the dispersion relation (16) contain several arbitrary constants, most of which can be easily related to the parameters (including the characteristic quantities) in the recursion method by the equivalences between equations (6a) and (19a), between (5) and (19b) and between (7) with (8) and (18). They are tabulated in table 2. Note that α cannot be uniquely determined when we fix the support E but do not fix the band shape.

Table 2. The correspondence of the parameters in the Toda lattice and in the recursion method.

Toda lattice	k or $q^{(a)}$	n (mass index)	$\mathrm{e}^{-C/2}$	V	κ	$-\omega t+\delta^{(b)}$	sign of ω
Recursion method	$E^{(a)}$	n (step index)	γ	λ_1	q_1 (or q_2)$^{(c)}$	α (or $-\alpha$)$^{(c)}$	$+$ (or $-$)$^{(c)}$

(a) This is not a quantitative correspondence.
(b) Note that δ is arbitrary. If we impose the direct correspondence between equations (18) and (7) with (8), then this item should be $-\omega t+\delta-\frac{1}{2}\kappa$.
(c) If we choose q_2 instead of q_1 (note $q_1+q_2=2\pi$), then the last two items are $-\alpha$ and $-$.

The only unsettled constant in equations (16)-(18) is the nome q of the theta functions. To determine this we may use the second-degree relation (6b). If we substitute equations (17) into equation (6b) and replace the sum by the integral (see § 4.1), then the nome q in equations (16)-(18) will be expressed as a function of the parameters in the recursion method. This procedure, however, seems to have no prospect of a simple and lucid expression, and is not followed here. In this paper we settle this nome by taking the following steps.

(i) First we express the characteristic quantities in the recursion method by use of the elliptic functions with an adequate parameter (modulus or nome). This parameter is written as a function of E, i.e. that of the band edges, and has at this moment nothing to do with the nome in equations (16)-(18).

(ii) Next we *assume* that the unsettled nome in equations (16)-(18) is given by the parameter used in step (i). Then equations (17), namely prospective analytic expressions for the asymptotic recursion coefficients, can be written in simple forms.

(iii) Lastly we prove that these expressions satisfy equation (6*b*).

The modulus (or the nome) in step (i) is, of course, not uniquely determined, since it is introduced only to express elliptic integrals. We must thus make a judicious choice.

We start with step (i). As mentioned in I, we need to calculate definite elliptic integrals such that the integrand contains a factor of $|(x-A_1)(x-A_2)(x-B_1)\times(x-B_2)|^{1/2}$. Then q_1 and s_1 are obtained by complete integrals of the third kind, and γ is obtained by incomplete ones of the third kind. Hence q_1 and s_1 are expressed by sn u (or cn u) and $Z(u)$, and γ is by $\theta_4(v)$ in addition (see Erdélyi 1953, pp 321, 363). Then the calculations are straightforward but tedious, and the resultant expressions are as follows.

For brevity we let

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

$$A = \tfrac{1}{4}(A_1 + B_1 + A_2 + B_2) \qquad W = \tfrac{1}{2}(w_1 + w_2) + g$$

and use the modulus k given by

$$k = [g(w_1 + w_2 + g)/(w_1 + g)(w_2 + g)]^{1/2}. \tag{20}$$

This choice of k is natural (see Erdélyi 1953, p308), and is indeed adequate for step (iii) as will be shown later. We also use the notations

$$q_1^* = (K/\pi)q_1$$

$$u_n^* = (K/\pi)u_n \qquad u_n = nq_1 + \alpha.$$

Then q_1 is determined by

$$c \equiv \text{cn}\ q_1^* = \tfrac{1}{2}(w_2 - w_1)/W \tag{21a}$$

and s_1 and γ are written by using q_1 as

$$s_1 = A + \tfrac{1}{2}W[cd + sZ(q_1^*)] \tag{22}$$

$$\gamma = \tfrac{1}{2}W\theta_4(0)/\theta_4(q_1/2\pi). \tag{23}$$

The nome in equation (23) is, of course, the one that corresponds to the k given by equation (20). We have introduced the abridged notations c, s and d, the latter two of which are defined by

$$s \equiv \text{sn}\ q_1^* = [(w_1 + g)(w_2 + g)]^{1/2}/W \tag{21b}$$

$$d \equiv \text{dn}\ q_1^* = \tfrac{1}{2}(w_1 + w_2)/W. \tag{21c}$$

The similar but different notations should be distinguished: s is defined by equation (21*b*), while s_1 is used to denote the saddle point. Note that $Z(u)$ is odd and periodic with period $2K$, while $\theta_4(v)$ is even and with period unity.

Now we *assume* (step (ii)) that both the nome in equations (16)-(18) and the modulus given by equation (20) represent the same parameter. Then the expressions (17) with equation (16) can be rewritten in simple forms as follows. Hereafter we mean the asymptotic a_n and b_n simply by a_n and b_n, respectively.

First we give the Fourier expansions (q expansions)

$$a_n - \lambda_1 = (2\pi/K)[(w_1+g)(w_2+g)]^{1/2} \sum_{j=1}^{\infty} q^j(1-q^{2j})^{-1} \sin(\tfrac{1}{2}jq_1)\cos[j(u_n - \tfrac{1}{2}q_1)]$$
$$\ln(b_n/\gamma) = 4\sum_{j=1}^{\infty} j^{-1}q^j(1-q^{2j})^{-1}\sin^2(\tfrac{1}{2}jq_1)\cos(ju_n) \tag{24}$$

which are the desired results (see equations (7) and (8) noting that α is arbitrary). The q expansions (24), which are known as rapidly converging Fourier series unless the modulus k is very close to unity, confirm the numerical observation that the asymptotic coefficients are well approximated by the constant and the principal terms (also see § 5.2).

Next the expressions in terms of the Jacobian functions are written as

$$a_n = \tfrac{1}{2}(A_1+B_2) + \tfrac{1}{2}g + w_2\left\{1 - \left[1 - \left(\frac{g}{w_2+g}\right)\operatorname{sn}^2(u_n^* - \tfrac{1}{2}q_1^*)\right]^{-1}\right\} \tag{25a}$$
$$b_n = \tfrac{1}{2}W\,\Delta_n^{1/2} \tag{25b}$$

after some tedious calculations. Here we have introduced a function

$$\Delta(u) \equiv 1 - k^2s^2\operatorname{sn}^2 u = 1 - [g(w_1+w_2+g)/W^2]\operatorname{sn}^2 u$$

which is even and periodic with period $2K$, and have written it simply as $\Delta_n \equiv \Delta(u_n^*)$.

Lastly we give alternative expressions for a_n. It is obvious that each expression must have a peculiar symmetric property with respect to the exchange of two subbands. That is to say, when w_1 and w_2 are exchanged for each other and α is replaced by $-\alpha$, then

(i) q_1 should be replaced by $2\pi - q_1$, and thus u_n by $-u_n \pmod{2\pi}$,
(ii) k, γ and b_n should be invariant, and
(iii) $s_1 - A$ $(= -(\lambda_1 - A))$ and $a_n - A$ should change their signs only.

These properties are apparent except for equation (25a), which is the expression that is convenient to see the upper and the lower bounds of a_n. To ascertain an apparently antisymmetric expression for $a_n - A$, we should observe the phases of a_n and $\ln b_n$. From the Fourier expansions (24) we see that the phases of $a_n \pm a_{n+1}$ and b_n are common to each other, and that the same is the case with those of a_n and $b_{n-1}b_n$. From these viewpoints we have

$$a_n^+ = \tfrac{1}{2}(a_n + a_{n+1}) = A - \tfrac{1}{2}Wcd/\Delta_n \tag{26}$$
$$a_n^- = \tfrac{1}{2}(a_n - a_{n+1}) = \tfrac{1}{2}Wk^2s^3\operatorname{sn}u_n^*\operatorname{cn}u_n^*\operatorname{dn}u_n^*/\Delta_n = -\tfrac{1}{4}Ws\,\Delta_n'/\Delta_n \tag{27}$$
$$(a_n^-)^2 = \tfrac{1}{4}W^2(1-\Delta_n)(1-d^2/\Delta_n)(1-c^2/\Delta_n) \tag{28}$$
$$a_n = A + \tfrac{1}{4}(W/cd)[\Delta_{n-1}\Delta_n - (c^2d^2 + c^2 + d^2)] \tag{29}$$

where $\Delta_n' \equiv \Delta'(u_n^*)$ (derivative).

We can now prove (step (iii)) that equation (6b) is satisfied, as given in appendix 2, and the analytic expressions obtained in this subsection are completely ascertained.

5. Miscellaneous remarks

5.1. Immediate consequences of the analytic expressions

The upper and the lower bounds of the asymptotic recursion coefficients can be easily obtained from equations (25a) and (25b). We denote them by the subscripts sup and inf for the upper and the lower bounds, respectively. Then we may obtain

$$\begin{aligned} a_{\mathrm{sup}} &= \tfrac{1}{2}(A_1 + B_2) + \tfrac{1}{2}g & a_{\mathrm{inf}} &= \tfrac{1}{2}(A_1 + B_2) - \tfrac{1}{2}g \\ b_{\mathrm{sup}} &= \tfrac{1}{4}(w_1 + w_2) + \tfrac{1}{2}g & b_{\mathrm{inf}} &= \tfrac{1}{4}(w_1 + w_2). \end{aligned} \tag{30}$$

In the commensurate case these bounds are not necessarily infinitesimally approached by the recursion coefficients. In the incommensurate case, on the other hand, they are equal to the superior and the inferior limits of the recursion coefficients, and thus we can obtain their rough estimates by such a plot as figure 1.

The expressions (26) and (29) indicate that a_n^+ is linearly related to $1/b_n^2$, and that a_n is linearly related to $b_{n-1}^2 b_n^2$, respectively. These relations and the estimates (30) were already obtained in the commensurate case by Turchi *et al* (1982) in different manners, i.e. they investigated the periodic linear chain by the Bloch theorem.

5.2. Numerical tests of the Fourier coefficients

In this subsection we compare our analytic results with numerical ones. For this purpose we examine the Fourier coefficients. The analytic results are given by equations (24) and the numerical ones are obtained by a simple procedure: the least squares fit of the asymptotic recursion coefficients to the forms

$$a_n \simeq C_0^a + \sum_{j=1}^{3} C_j^a \cos\{j[(n-\tfrac{1}{2})q_1 + \alpha_j^a]\}$$

$$\ln b_n \simeq C_0^b + \sum_{j=1}^{3} C_j^b \cos[j(nq_1 + \alpha_j^b)].$$

This fit is done over the last 30 recursion coefficients shown in figure 1 (i.e. for $30 \leqslant n \leqslant 59$).

The results are listed in table 3. Note that the numerical C_3^a is chosen to be negative in accordance with the analytic estimate, and that $\alpha_j^{a/b}/2\pi$ has an ambiguity in modulus

Table 3. Comparison of the analytic and the numerical estimates of the first Fourier coefficients. The numerical estimates are based on the recursion coefficients shown in figures 1(a–d). For each estimate the upper figure indicates C_j^a or $\alpha_j^a/2\pi$ and the lower figure indicates C_j^b or $\alpha_j^b/2\pi$.

Support		C_0	C_1	C_2	C_3	$\alpha_1/2\pi$	$\alpha_2/2\pi$	$\alpha_3/2\pi$
E_1	Analytic	1.738 73	0.502 52	0.011 39	−0.002 53	—	—	—
$k^2 = 7/10$		−0.177 13	0.293 45	0.001 01	0.000 45	—	—	—
$q = 0.074\,690$	Numerical	1.738 76	0.502 17	0.011 36	−0.002 54	0.9511	0.9510	0.9500
	(figure 1(a))	−0.177 00	0.293 17	0.001 03	0.000 44	0.9510	0.9526	0.9476
	Numerical	1.739 12	0.502 89	0.011 62	−0.000 93	0.1728	0.1726	0.2196
	(figure 1(b))	−0.177 20	0.293 42	0.001 16	0.000 52	0.1726	0.1636	0.2199
E_2	Analytic	1.707 53	0.500 61	0.042 89	−0.000 58	—	—	—
$k^2 = 7/9$		−0.187 88	0.293 87	0.011 71	0.000 02	—	—	—
$q = 0.092\,927$	Numerical	1.707 59	0.500 32	0.042 95	−0.000 58	0.8454	0.8451	0.8475
	(figure 1(c))	−0.187 74	0.293 68	0.011 62	0.000 04	0.8454	0.8459	0.8827
	Numerical	1.707 87	0.500 44	0.043 19	−0.000 69	0.0152	0.0154	−0.0063
	(figure 1(d))	−0.187 90	0.293 82	0.011 46	0.000 17	0.0151	0.0141	0.0032

$1/j$. We observe that these Fourier series are no doubt rapidly converging. The phase constant cannot be determined analytically as far as this paper is concerned, but we have the analytic assertion that all the α_j^a and α_j^b for each particular band shape should be equal to one another. We may find good agreements in the whole range of the comparisons. The distinguishable deviations of $\alpha_3^{a/b}$ in some cases are inevitable, since the corresponding $C_3^{a/b}$ are very small.

5.3. *The inverse problem*

First we refer to the familiar problem: what spectrum is produced by the periodic recursion coefficients? Suppose that no condition is imposed but that they are periodic. The answer is well known. If the period is integer, say p, then the corresponding spectrum is in general composed of p subbands, which are all absolutely continuous. In the incommensurate case, on the other hand, a singularly continuous spectrum occurs in general (see Cycon *et al* 1987).

Our problem, where the spectrum is given first, can be regarded as the inverse of the above problem, where the coefficients are given first. The above-mentioned general properties of the spectral structures should be compared with the following result of our problem. If the periodic a_n and b_n are written in the forms of equations (25a) and (25b), then the spectrum is always composed of two absolutely continuous subbands (and an additional point spectrum may exist) no matter what their period may be (two, three, ..., or even infinity (incommensurate)).

5.4. *Single band as a limiting case*

It is obvious that we can construct the single-band case by taking an adequate limit of our two-band case. We are reminded of two kinds of such limits. One is $g \to 0$ (then $k \to +0$), and the other is w_1 (or w_2) $\to 0$ (then $k \to 1-0$).

The former limiting case is rather trivial. We note that $a_{\sup} - a_{\inf} = g$ and $b_{\sup} - b_{\inf} = \frac{1}{2}g$, i.e. the amplitudes (in the general incommensurate case) of the asymptotic oscillations of a_n and b_n are proportional to g. Thus the limit $g \to 0$ directly implies the convergence of a_n and b_n, from which a simple single-band case follows.

The latter limiting case, on the contrary, is not necessarily trivial. If we simply let $w_1 = 0$, then it is not apparent that the asymptotic a_n and b_n assume the single-band limiting values ($\frac{1}{2}(A_2 + B_2)$ and $\frac{1}{4}w_2$, respectively). We should consider the case where w_1 is infinitesimally small but not zero. Then q_1 is also infinitesimally small and we have a very large but not infinite period. We may assume that this period is in general incommensurate, and thus both the upper and the lower bounds (equations (30)) are significant as the superior and the inferior limits, respectively. They are given by $a_{\inf} = \frac{1}{2}(A_2 + B_2) + 0$, $a_{\sup} = a_{\inf} + g$, $b_{\inf} = \frac{1}{4}w_2 + 0$ and $b_{\sup} = b_{\inf} + \frac{1}{2}g$, and therefore the recursion coefficients have finite swings. We can relate this limiting case to a *soliton* in the corresponding Toda lattice. We know that a soliton solution follows from the long wavelength limit of the simply periodic motion in the Toda lattice (see Toda 1981). The finite differences between the upper and the lower bounds (g for a_n and $\frac{1}{2}g$ for b_n) correspond to the height of the soliton.

5.5. *Multigap cases*

Although our explicit expressions apply to the single-gap case only, we can treat the general multigap cases in the same manner as in § 4. More generalised wave-like solutions of the Toda lattice are already known, and are expressed in terms of the Riemannian theta functions (Date and Tanaka 1976). These solutions in general give almost periodic waves and correspond to the asymptotic recursion coefficients in the multigap cases. The explicit forms are not given here and will be discussed elsewhere.

6. Conclusions

In this paper we intended to ascertain the asymptotic forms of the recursion coefficients in the two-band (single-gap) case, and have succeeded in expressing them by use of the elliptic functions, except that there remains a single parameter α (phase constant of the asymptotic oscillations) unsettled. The resultant expressions are written as functions of the support, except for this phase constant that depends on the band shape.

These expressions are derived through the mathematical connection between the recursion method and the Toda lattice, which seems to be somewhat surprising. This connection, which is significant in the multiband cases rather than in the single-band case, may promise well for a deeper understanding of the recursion method, since the Toda lattice has been investigated to a large extent. We may state that the result in this paper is a typical example of the benefits of this connection.

Appendix 1. Functions subject to the C-free condition

The C-free condition given in § 4.1 seems at first sight to be too restrictive. As a matter of fact, however, we can easily construct a function that satisfies this condition as follows.

We denote the C-free function by the same notation $F(nq_1+\alpha; E)$ as in the main text (a superscript is omitted), and for simplicity consider the case where the second argument is q_1. Then the C-free condition becomes

$$\frac{1}{p}\sum_{j=0}^{p-1} F((2\pi/p)j+\alpha;\, q_1=2\pi r/p)=\frac{1}{2\pi}\int_0^{2\pi} F(x;\, q_1)\,\mathrm{d}x \tag{A1.1}$$

where r/p is an arbitrary fraction and is assumed to be irreducible. Since $F(x; q_1)$ is periodic concerning x with period 2π, we expand it in the Fourier series

$$F(x;\, q_1)=\sum_{m=-\infty}^{\infty} f_m(q_1)\,\mathrm{e}^{\mathrm{i}mx} \tag{A1.2}$$

and substitute it into equation (A1.1). Then the sums over j in the left-hand side vanish except for the terms where m is an integral multiple of p, and we may obtain

$$\sum_{k(\neq 0)}{}' f_{kp}(2\pi r/p)\,\mathrm{e}^{\mathrm{i}kp\alpha}=0$$

where the summation is over non-zero integers. Since α should be regarded as arbitrary, we have

$$f_m(2\pi r/p)=0 \qquad \text{for } m=\pm p,\ \pm 2p,\ \pm 3p, \ldots. \tag{A1.3}$$

This condition is satisfied if $f_m(q_1)=0$ for every m such that $mq_1=0\ (\mathrm{mod}\ 2\pi)$ and $m\neq 0$. The simplest example is $f_m(q_1)=\sin\frac{1}{2}mq_1$. The Fourier expansions (24) of a_n and $\ln b_n$ evidently satisfy the condition (A1.3).

Appendix 2. Proof of the relation (6*b*)

We introduce the definite integrals defined by

$$I_n = \frac{1}{2K}\int_0^{2K} [\Delta(u)]^n \mathrm{d}u$$

and express all the quantities by A, W, s, c, d and I_n. Then the band edges are written as

$$\begin{aligned} A_1 &= A+\tfrac{1}{2}W(1-c+d) \qquad & B_1 &= A+\tfrac{1}{2}W(1+c-d) \\ A_2 &= A+\tfrac{1}{2}W(-1+c+d) \qquad & B_2 &= A+\tfrac{1}{2}W(-1-c-d). \end{aligned} \tag{A2.1}$$

We can derive the recurrence relation

$$2n\,c^2d^2I_{n-1}-(2n+1)(c^2d^2+c^2+d^2)I_n+(2n+2)(1+c^2d^2)I_{n+1}-(2n+3)I_{n+2}=0 \tag{A2.2}$$

and we may obtain

$$I_0=1 \qquad I_{-1}=1+(s/cd)Z(q_1^*).$$

The value of I_1, which enables us to know all of I_n, is not necessary here. The saddle point s_1 is thus written as

$$s_1=A+\tfrac{1}{2}Wcd\,I_{-1}. \tag{A2.3}$$

Now it is straightforward to prove that the expressions given in § 4.4 satisfy equation (6*b*) provided that we use equations (26)-(28) for a_n and equation (25*b*) for b_n. We rewrite the summand in the left-hand side of equation (6*b*) as $(a_j^+)^2+2a_j^+a_j^-+(a_j^-)^2+2b_j^2$, substitute equations (25*b*) and (26)-(28), and replace the limiting arithmetic mean by the integral. Here note that it has already been implicitly proved that the summand satisfies the C-free condition, since this mean corresponds to a constant of motion (the energy conservation) in the Toda lattice irrespective of the commensurability. Then the integral of the second term $2a_j^+a_j^-$ evidently vanishes (see equation (27)), and those of the other terms can be expressed by I_n (use equation (28) for the third term $(a_j^-)^2$). The left-hand side is then equal to $A^2-AWcd\,I_{-1}+\frac{1}{4}W^2(1+c^2+d^2)$, where use is made of the recurrence relation (A2.2) (let $n=-1$). The right-hand side of equation (6*b*) is, on the other hand, easily evaluated by equations (4*b*), (A2.1) and (A2.3), and we see that both the sides are equal to each other.

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