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Contents

Notes on the Rate of Convergence of the Rayleigh-Ritz and Weinstein-Bazley Methods

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1. Introduction

It is of considerably difficult problem to estimate the rate of convergence of the Rayleigh-Ritz(RR) and the Weinstein-Bazley(WB) methods applied to general self-adjoint operators. For a certain class of operators, however, it can be easily estimated by comparing the corresponding matrices. The purpose of this note is to show this for the finite Hill operator and give some observations for another operator .

Let A be a self-adjoint operator in a real Hilbert space having the inner product (,) and the norm $\|u\|=\sqrt{(u,u)}$. We assume that A is bounded below and that its spectrum consists of isolated eigenvalues $\lambda_1\leq\lambda_2\leq\ldots$ each having finite multiplicity. Further we assume that A can be represented as $A^{(0)}+A'$, where $A^{(0)}$ is a self-adjoint operator with known discrete eigenvalues $\lambda_i^{(0)}$ $(\lambda_1^{(0)}\leq\lambda_2\leq\ \ldots)$ and known orthonormal eigenfunctions $u_i^{(0)}$. We denote by $\Lambda_i^{(n)}(\Lambda_1^{(n)}\leq\Lambda_2^{(n)}\leq\ \ldots\leq\Lambda_n^{(n)})$ and $r_i^{(n)}={}^t(r_{i1}^{(n)},\ldots,r_{in}^{(n)})$ be the eigenvalues and the orthonormal eigenvectors of the n×n RR matrix $R_n=(Au_i^{(0)},u_j^{(0)})$ based upon the test functions $u_1^{(0)},\ldots,u_n^{(0)}$. $\lambda_i^{(n)}(\lambda_1^{(n)}\leq\ \ldots\leq\lambda_n^{(n)})$ and $w_i^{(n)}={}^t(w_{i1}^{(n)},\ldots,w_{in}^{(n)})$ stand for the eigenvalues and the orthonormal eigenvectors of the WB matrix $W_n=(\lambda_i^{(0)}\delta_{ij})+([p_i,p_j])^{-1}$ respectively, where $p_i= A'^{-1}u_i^{(0)}$ (Bazley's special choice) and $[u,v]=(A'u,v)$ for $u,v\in D(A')$, the domain of A'. It is known that, if $\lambda_n^{(n)}\leqq\lambda_{n+1}^{(0)}$, $\lambda_i^{(n)}\leqq\lambda_i^{(n+1)}\leqq\lambda_i\leqq\Lambda_i^{(n+1)}\leqq\Lambda_i^{(n)}$ for each $i\leqq n$. $U_i^{(n)}=\sum_{j=1}^{n} r_{ij}^{(n)}u_j^{(0)}$ and $u_i^{(n)}=\sum_{j=1}^{n} w_{ij}^{(n)}u_j^{(0)}$ give the RR and WB approximations for the orthonormal eigenfunction u_i corresponding to λ_i, respectively.

2. The Matrices R_n and W_n for a Certain Class of Operators

We first state the following theorem.

Theorem 1. Let

(1) $$A'u_i^{(0)}=\sum_{j=1}^{i+L}\beta_{ij}u_j^{(0)} \quad (i=1,2,\ldots,n)$$

for some scalar β_{ij}. Then $R_n-W_n=(\varepsilon_{ij}^{(n)})$ where $\varepsilon_{ij}^{(n)}=0$ if $i\leqq n-L$ or $j\leqq n-L$.

Proof. We first note that $\beta_{ij}=(A'u_i^{(0)},u_j^{(0)})=\beta_{ji}$ and that the conditions (1) are equivalent to

$$A'u_i^{(0)}=\sum_{k=i-L}^{i+L}\beta_{ik}u_k^{(0)} \quad (i=1,2,\ldots,n)$$

or

$$u_i^{(0)}=\sum_{k=i-L}^{i+L}\beta_{ik}p_k.$$

Hence we have $\delta_{ij}=(u_i^{(0)},u_j^{(0)})=\sum_{k=i-L}^{i+L}\beta_{ik}(p_k,u_j^{(0)})=\sum_{k=i-L}^{i+L}\beta_{ik}[p_k,p_j]$.

This implies that, for each i such that $i\leqq n-L$, the vector $(\overbrace{0,\ldots,0}^{i-L-1},\beta_{ii-L},\ldots,\beta_{ii+L},\overbrace{0,\ldots,0}^{n-i-L})$ (or its transpose) gives the i-th row (or column) of the n×n matrix $(b_{ij})=([p_i,p_j])^{-1}$. In order to determine the other elements $b_{\sigma\tau}$, we put $b_{\sigma\tau}=\beta_{\sigma\tau}-\varepsilon_{\sigma\tau}^{(n)}$ $(\sigma,\tau=n-L+1,\ldots,n)$. Then, substituting the relation

$$\sum_{k=\tau-L}^{\tau+L}[p_\sigma,p_k]\beta_{k\tau}=\delta_{\sigma\tau}$$

into

$$\sum_{k=\tau-L}^{n-L}[p_\sigma,p_k]\beta_{k\tau}+\sum_{k=n-L+1}^{n}[p_\sigma,p_k](\beta_{k\tau}-\varepsilon_{k\tau}^{(n)})=\delta_{\sigma\tau},$$

we now obtain

$$(2)\qquad \sum_{k=n-L+1}^{n}[p_\sigma,p_k]\varepsilon_{k\tau}^{(n)}=-\sum_{k=n+1}^{\tau+L}[p_\sigma,p_k]\beta_{k\tau}\quad(\sigma=1,2,\ldots,n).$$

Clearly the system (2) has the unique solution $\varepsilon_{j\tau}^{(n)}(n-L<j\leq n)$ for each $\tau(n-L<\tau\leq n)$, and (2) is equivalent to

$$(3)\qquad \sum_{k=n-L+1}^{n}[p_\sigma,p_k]\varepsilon_{k\tau}^{(n)}=-\sum_{k=n+1}^{\tau+L}[p_\sigma,p_k]\beta_{k\tau}\quad(\sigma=n-L+1,\ldots,n).$$

This completes the proof. Q.E.D.

3. The Rate of Convergence of the Methods Applied to the Finite Hill Equation

In this section we shall apply Theorem 1 to estimate the rate of convergence of the RR and WB methods applied to the finite Hill equation. Let A be defined by

$$Au=-u''+\left(\sum_{k=1}^{L}2c_{2k}\cos 2kx\right)u,\quad c_{2L}\neq 0,$$

where the domain of A consists of the functions u such that $u(0)=u(\pi)=0$, $u(x+\pi)=u(x)$, u' is absolutely continuous and $u''\in L^2(0,\pi)$. We define the operators $A^{(0)}$ and A' as

$$A^{(0)}u=-u''+\alpha u,\quad A'=A-A^{(0)}$$

respectively, where α is a constant such that $\alpha>M\equiv\sum_{k=1}^{L}2|c_{2k}|$. Then

$$\lambda_i^{(0)}=4i^2-\alpha,\quad u_i^{(0)}=\sqrt{\frac{2}{\pi}}\sin 2ix\quad(i\geq 1).$$

Therefore the conditions (1) are satisfied with

$$\beta_{ij}=\alpha\delta_{ij}+\sum_{k=1}^{L}c_{2k}(\delta_{i-j,k}-\delta_{i+j,k}).$$

Lemma 1. Let A be the operator defined as above. Then there exists a positive constant ε independent on n such that $|\varepsilon_{ij}^{(n)}| \leq \varepsilon$ $(n-L<i,j\leq n)$ for all n.

Proof. We rewrite (3) in the matrix form

(4) $\quad ([p_{n-L+i}, p_{n-L+j}])(\varepsilon^{(n)}_{n-L+i;n-L+j}) = -([p_{n-L+i}, p_{n+j}])C$

$(i,j=1,2,\ldots,L),$

where

$$C = \begin{pmatrix} \beta_{n+1,n-L+1} & \cdots & \beta_{n+1,n} \\ & \ddots & \vdots \\ 0 & & \beta_{n+L,n} \end{pmatrix} = \begin{pmatrix} c_{2L} & c_{2L-2} & \cdots & c_2 \\ & \ddots & \ddots & \vdots \\ & & \ddots & c_{2L-2} \\ 0 & & & c_{2L} \end{pmatrix}.$$

As is easily seen, we have

$$[p_{n-L+i}, p_{n-L+j}] = \frac{2}{\pi}\int_0^\pi \phi(x)\sin 2(n-L+i)x \sin 2(n-L+j)x dx$$

$$\rightarrow \frac{1}{\pi}\int_0^\pi \phi(x)\cos 2(i-j)x\, dx \equiv p_{ij}$$

and

$$[p_{n-L+i}, p_{n+j}] \quad \rightarrow \frac{1}{\pi}\int_0^\pi \phi(x)\cos 2(j-i+L)x\, dx \equiv q_{ij}$$

as $n\rightarrow\infty$, where $\phi(x) = (\alpha+2\sum_{k=1}^{L} c_{2k}\cos 2kx)^{-1}$. Further we can show that, if α is sufficiently large (e.g., $\alpha > M + \frac{LM^2}{2|c_{2L}|}$), the L×L matrix $P=(p_{ij})$ is strictly diagonally dominant, and nonsingular. Therefore we conclude from (4) that

$$(\varepsilon^{(n)}_{n-L+i,n-L+j}) \rightarrow -P^{-1}QC$$

as $n\rightarrow\infty$, where $Q=(q_{ij})$ $(i,j=1,2,\ldots,L)$. Q.E.D.

From Lemma 1 and the relation $W_n w_i^{(n)} = \lambda_i^{(n)} w_i^{(n)}$, we have

Lemma 2. Let $k \geq 1$ be fixed and m be any positive integer such that $n-mL \to \infty$ as $n \to \infty$. Then we have

$$w_{kj}^{(n)} = o\left(\left\{\frac{\hat{M}\sqrt{L}}{4(n-mL)^2}\right\}^m\right)$$

$$(j=n-L+1, n-L+2, \ldots, n),$$

$$w_{n-k,j}^{(n)} = O\left(n^{-[\frac{k}{L}]}\right)$$

where

$$\hat{M} = M + 2(L-1)\varepsilon.$$

Therefore, by the same way as in the previous paper[16], we can apply Wilkinson's result[15;pp.172-173] to estimate the rate of convergence of the RR and WB methods. The results are stated without proofs as follows:

Theorem 2. Under the same assumption as in Lemma 2, we have

$$\Lambda_k^{(n)} - \lambda_k^{(n)} = o\left(\left\{\frac{\hat{M}\sqrt{L}}{4(n-mL)^2}\right\}^{2m}\right)$$

$$\Lambda_{n-k}^{(n)} - \lambda_{n-k}^{(n)} = O\left(n^{-2[\frac{k}{L}]}\right)$$

$$\Lambda_n^{(n)} - \lambda_n^{(n)} \leq L^2\varepsilon.$$

Corollary 1. $\Lambda_k^{(n)} - \lambda_k^{(n)} = o\left(\left\{\frac{\hat{M}\sqrt{L}}{n^2}\right\}^{2[\frac{n}{2L}]}\right).$

Theorem 3. Let $(u_k^{(n)}, u_k) \geq 0$ for fixed k. Then, as $n \to \infty$, we have

$$\| u_k^{(n)} - u_k \| = o\left(\left\{\frac{\hat{M}\sqrt{L}}{4(n-mL)^2}\right\}^m\right) \quad (k \geq 1,\ n-mL \to \infty)$$

$$\|u_{n-k}^{(n)} - u_{n-k}\| = O(n^{-[\frac{k}{L}]-1}) \quad (k\geq 0).$$

Corollary 2. $\|u_k^{(n)} - u_k\| = o(\left\{\frac{\hat{M}\sqrt{L}}{n^2}\right\}^{[\frac{n}{2L}]})$.

Theorem 4. Take the vectors $w_i^{(n)}$ and $r_i^{(n)}$ so as to satisfy $\sum_{\sigma,\tau=n-L+1}^{n} \varepsilon_{\sigma,\tau}^{(n)} w_{i\sigma}^{(n)} r_{i\tau}^{(n)} > 0$ for all n. Then, for fixed k, we have, as $n\to\infty$,

$$\|U_k^{(n)} - u_k\| = o(\left\{\frac{\hat{M}\sqrt{L}}{4(n-mL)^2}\right\}^m) \quad (k\geq 1,\ n-mL\to\infty)$$

$$\|U_{n-k}^{(n)} - u_{n-k}\| = O(n^{-[\frac{k}{L}]-1}) \quad (k\geq 0).$$

Corollary 3. $\|U_k^{(n)} - u_k\| = o(\left\{\frac{\hat{M}\sqrt{L}}{n^2}\right\}^{[\frac{n}{2L}]})$.

Remark. We can prove that $\sum_{\sigma,\tau=n-L+1}^{n} \varepsilon_{\sigma\tau}^{(n)} w_{i\sigma}^{(n)} w_{i\tau}^{(n)} > 0$ for any n and i such that $n>L$ and $1\leq i\leq n$. Therefore the assumption of Theorem 4 will be satisfied for sufficiently large n.

4. Observation for the Other Equation

Consider an operator A defined by

$$Au= -u'' + q(x)u, \quad u(x)=u(-x), \quad u(x)\in L^2(-\infty,\infty)$$

where q(x) is a polynomial of degree 2L such that $q(x)>x^2-\alpha$ for some constant $\alpha>0$ and $q(-x)=q(x)$. (The case of $q(x)=x^2+ax^4$ $(0<a<1)$ has been treated by Bazley and Fox[2].) Then $A^{(0)}u= -u''+(x^2-\alpha)u$ and $A'=A-A^{(0)}$ are suitable decomposition. We have

$$\lambda_i^{(0)} = 4i-3-\alpha,$$

$$u_i^{(0)} = \frac{1}{2^{i-1}\sqrt{(2i-2)!\sqrt{\pi}}} e^{-\frac{x^2}{2}} H_{2i-2}(x) \quad (i \geqq 1),$$

where

$$H_m(x) = (-1)^m e^{x^2} \frac{d^m}{dx^m} e^{-x^2} \quad \text{(the m-th Hermite polynomial).}$$

By the reccurence relation $2xH_m = 2mH_{m-1} + H_{m+1}$ or

$$(5) \quad 2x^2 u_i^{(0)} = \sqrt{(2i-2)(2i-3)}\, u_{i-1}^{(0)} + (4i-3) u_i^{(0)} + \sqrt{2i(2i-1)}\, u_{i+1}^{(0)},$$

we see that the conditions (1) are satisfied. Further we have

$$[p_\sigma, p_\tau] = \frac{1}{2^{\sigma+\tau-2}\sqrt{(2\sigma-2)!(2\tau-2)!\pi}} \int_{-\infty}^{\infty} \frac{e^{-x^2} H_{2\sigma-2} H_{2\tau-2}}{q(x)-x^2+\alpha} dx$$

$$= O(1)$$

since

$$|H_m(x)| \leqq e^{\frac{x^2}{2}} \sqrt{2^{m+1}} \sqrt{m!}.$$

On the other hand, the relation (5) shows that $\beta_{ij} = O(i^L)$. Hence, if n is large, we may roughly conclude from (4) that $\varepsilon_{ij}^{(n)} = O(n^L)$ $(n-L+1 \leqq i, j \leqq n)$. Therefore, even if the methods are convergent, the rate of convergence in this case may be rather slow, compared with the case of the finite Hill operator. The more precise information will be given elsewhere.

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On the Superiority of the Trapezoidal Rule for the Integration of Periodic Analytic Functions

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§1 Introduction

It is well-known that the trapezoidal rule with an equal mesh size yields a result with remarkably high accuracy when applied to the integration of a periodic analytic function over its period. Frequently this rule is even called the "best" rule with rather vague definition of the word "best". Several attempts seem to have been made to show the "best" property of the trapezoidal rule (e.g.[1]) by comparing the results with other various well-known formulas such as Gauss rules.

In the present paper we will define the best rule for numerical integration of periodic analytic functions over its period in terms of the asymptotic decay rate of the exponent of the characteristic function of the error [3], and show that the trapezoidal rule is the best under this definition in the similar way as in the preceding paper [3].

§2 The complex integral representation of the error

Let f(x) be analytic over [a,b] and periodic with period b-a. We consider the integral of f(x) over its period:

$$I = \int_a^b f(x)dx \qquad (2.1)$$

We write an approximate formula for (2.1) as follows:

$$I_n = \sum_{k=1}^{n} A_k f(a_k) \quad , \tag{2.2}$$

where a_k and A_k are the sampling points and the weights, respectively. The error $\Delta I_n = I - I_n$ of (2.2) can be expressed in the form of a complex integral:

<u>Theorem 1</u> Let f(x) be analytic over [a,b] and periodic with period b-a. Then

$$\Delta I_n = \int_a^b f(x)dx - \sum_{k=1}^{n} A_k f(a_k)$$
$$= \frac{1}{2\pi i}\int_C \Psi(z)f(z)dz - \frac{1}{2\pi i}\int_C \Psi_n(z)f(z)dz \tag{2.3}$$

where

$$\Psi(z) = \begin{cases} -\pi i \ ; & \text{Im } z > 0 \\ \pi i \ ; & \text{Im } z < 0 \end{cases} \tag{2.4}$$

$$\Psi_n(z) = \sum_{m=-\infty}^{\infty}\{\sum_{k=1}^{n} A_k\left(\frac{1}{z-a_k-m(b-a)} + \frac{1}{a_k+m(b-a)}\right)\} \ . \tag{2.5}$$

The path C of the integral (2.3) consists of two line segments C_1 and C_3 parallel to the real axis as shown in Fig.1 and is taken in such a way that there exists no singular point of f(z) between the two line segments.

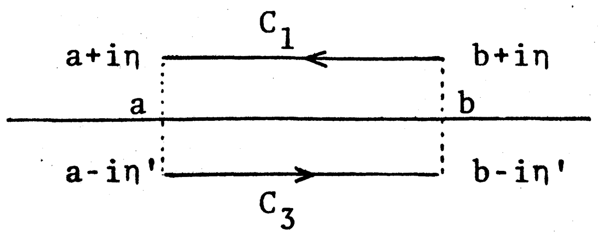


Fig.1 The path C of the integral (2.3)

Proof The first term of (2.3) is evident since, if we deform the path by letting $\eta\to 0$ and $\eta'\to 0$, then we have

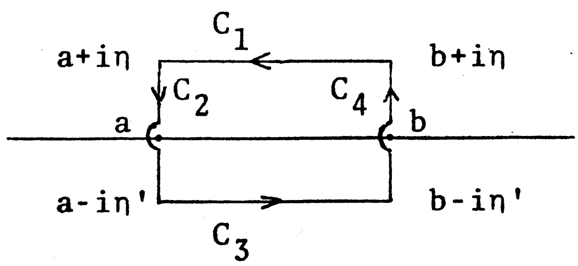
$$\frac{1}{2\pi i}\int_C \Psi(z)f(z)dz = \int_a^b f(x)dx \quad . \tag{2.6}$$

It can be seen that the right hand side of (2.5) converges uniformly on compact sets not containing any of the poles and defines a meromorphic function. Since $f(z)$ and $\Psi_n(z)$ are both periodic, $\Psi_n(z)f(z)$ is also periodic with period b-a so that we can join the lines C_1 and C_3 with no change of ΔI_n by two line segments C_2 and C_4 parallel to the imaginary axis and form a rectangular contour C' with positive orientation. If a sampling point is located at the end point x=a or x=b, C_2 and C_4 are deformed slightly in such a way that they do not pass through the sampling point and that they have the same shape (Fig.2). Then from the residue theorem,

$$\frac{1}{2\pi i}\oint_{C'} \Psi_n(z)f(z)dz = \sum_{k=1}^{n} A_k f(a_k) \quad , \tag{2.7}$$

and we have (2.3) from (2.6), which completes the proof.

Fig.2 The path C'



We call

$$\Phi_n(z) = \Psi(z) - \Psi_n(z) \tag{2.8}$$

the characteristic function of the error [3]. In case of the trapezoidal rule with an equal mesh size of $h=(b-a)/n$, we have

$$\Phi_n(z) = \begin{cases} -\pi i - \pi\cot\frac{\pi}{h}z = \dfrac{-2\pi i}{1-\exp(-2\pi iz/h)} \; ; \; \mathrm{Im}\, z > 0 \\ \pi i - \pi\cot\frac{\pi}{h}z = \dfrac{+2\pi i}{1-\exp(+2\pi iz/h)} \; ; \; \mathrm{Im}\, z < 0 \end{cases} \tag{2.9}$$

with the aid of the partial fraction expansion of cotangent function. Note that $\Phi_n(z)$ of the trapezoidal rule has no zeros on the finite z-plane.

§3 Asymptotic decay rate of the exponent of the characteristic function and the best formula

When $\mathrm{Im}\, z \gg h$ in the upper half-plane, $\Phi_n(z)$ of (2.9) can be approximated by

$$|\Phi_n(z)| \simeq 2\pi\exp(-2\pi y/h), \quad y=\mathrm{Im}\, z \quad , \tag{3.1}$$

and hence the quantity

$$-\frac{\partial}{\partial y}\log|\Phi_n(x+iy)| \simeq \frac{2\pi}{h} \; , \quad z=x+iy \tag{3.2}$$

can be regarded to define the decay rate of the exponent of $|\Phi_n(z)|$ in the upper half-plane. Since $\Phi_n(\bar{z})=\overline{\Phi_n}(z)$, we will consider the decay rate only in the upper half-plane. It would intuitively be clear that $\Psi_n(z)$ of a useful formula must converge to $\mp\pi i$ as $\mathrm{Im}\, z\to\pm\infty$ with all its derivatives and that generally a formula having a larger decay rate of the exponent of the characteristic function results in a smaller error when applied to the integration of a certain fixed function. And hence the decay rate can be considered to be a criterion to define the best formula. Accordingly we define the average decay rate of the exponent of $|\Phi_n(z)|$ at a distance d from the real axis in the upper half-plane by

$$r(d) = -\frac{1}{b-a}\int_{a+id}^{b+id} \frac{\partial}{\partial y} \log|\Phi_n(z)|\,dz \,, \tag{3.3}$$

and define the *asymptotic decay rate* by

$$r = \lim_{d\to\infty} r(d) \quad . \tag{3.4}$$

Now we call a formula having the largest asymptotic decay rate *the best formula*.

Theorem 2 The trapezoidal rule with an equal mesh size is the best formula for the integration of a periodic analytic function over its period b-a among formulas having the same number of sampling points on [a,b).

Proof Consider an integral

$$J = -\frac{1}{2\pi i}\oint_{\Gamma} \frac{\Psi_n'(z)}{\pi i+\Psi_n(z)}\,dz \tag{3.5}$$

where $\Psi_n(z)$ is defined by (2.5). The path Γ is taken to be a rectanglar contour with positive orientation with corners at b+id, a+id, a-id' and b-id' as shown in Fig.3. When a

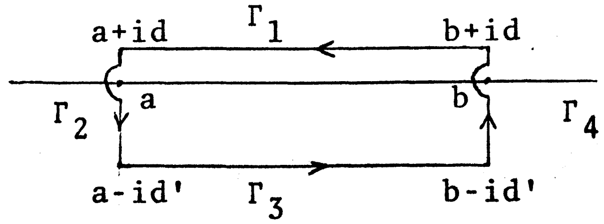


Fig.3 The path Γ of (3.5)

sampling point lies on x=a or on x=b, Γ is modified as in the proof of Theorem 1. Now n is the number of the sampling points. Note that n is nothing but the number of poles of $\pi i+\Psi_n(z)$ located inside Γ. Then from the principle of the argument we have

$$J = n - n_z \tag{3.6}$$

where n_z is the number of zeros of $\pi i+\Psi_n(z)$ inside Γ. Since $\Psi_n'(z)/\{\pi i+\Psi_n(z)\}$ is periodic with period b-a, the integrals along Γ_2 and Γ_4 cancel each other for any value of d and d'. Since $\Psi_n(z)$ must converge, on the other hand, to the constant function πi as $d'\to\infty$, the integral along Γ_3 can be made as small as one wishes by letting $d'\to\infty$. Hence we have

$$J = \frac{1}{2\pi i}\int_{a+id}^{b+id} \frac{d}{dz}\log\{\pi i+\Psi_n(z)\}dz \tag{3.7}$$

as $d'\to\infty$. Since $\log\{\pi i+\Psi_n(z)\}$ is analytic along Γ_1, we can replace d/dz by partial derivative $\partial/\partial x$ so that

$$\begin{aligned} J &= \frac{1}{2\pi i}\int_{a+id}^{b+id} \frac{\partial}{\partial x}[\log|\pi i+\Psi_n(z)|+i\arg\{\pi i+\Psi_n(z)\}]dz \\ &= \frac{1}{2\pi i}\int_{a+id}^{b+id} \{\frac{\partial}{\partial x}\log|\pi i+\Psi_n(z)|-i\frac{\partial}{\partial y}\log|\pi i+\Psi_n(z)|\}dz \\ &= \frac{1}{2\pi i}\int_{a+id}^{b+id} \frac{\partial}{\partial x}\log|\Phi_n(z)|dz \\ &\qquad - \frac{1}{2\pi}\int_{a+id}^{b+id} \frac{\partial}{\partial y}\log|\Phi_n(z)|dz \end{aligned} \tag{3.8}$$

in view of Cauchy-Riemann equation. We know that J is real from (3.6) and hence the first term of the right hand side of (3.8) is zero. Accordingly, by letting $d\to\infty$, we obtain an important relation between $n-n_z$ and the asymptotic decay rate r:

$$r = \frac{2\pi}{b-a}(n-n_z) \le \frac{2\pi n}{b-a} \tag{3.9}$$

This shows that the asymptotic decay rate r cannot be larger than $\frac{2\pi n}{b-a}$ and the maximum value $\frac{2\pi n}{b-a}$ is attained by such $-\pi i-\Psi_n(z)$ that satisfies $n_z=0$, i.e. that has no zeros in the finite z-plane, if such $-\pi i-\Psi_n(z)$ exists. We have, on the other hand, already seen that $-\pi i-\Psi_n(z)$ of the trapezoidal rule has no zeros in the finite z-plane, and hence the trapezoidal rule is the best formula, in which $r=\frac{2\pi n}{b-a}=\frac{2\pi}{h}$.

§4 Discussions

The characteristic function of the error of Simpson's formula

$$\begin{aligned} I_s &= \frac{h}{3}\{f(a)+4f(a+h)+2f(a+2h)+4f(a+3h)+\cdots +f(b)\} \\ &= \frac{4}{3}h\{\frac{1}{2}f(a)+f(a+h)+f(a+2h)+\cdots+\frac{1}{2}f(b)\} \\ &\quad -\frac{1}{3}(2h)\{\frac{1}{2}f(a)+f(a+2h)+f(a+4h)+\cdots+\frac{1}{2}f(b)\}\ , \quad h=\frac{b-a}{n} \end{aligned} \tag{4.1}$$

is given by

$$\Phi_s(z) = \begin{cases} -\pi i-\frac{4}{3}\pi\cot\frac{\pi}{h}z+\frac{1}{3}\pi\cot\frac{\pi}{2h}z & ; \quad \text{Im } z > 0 \\ \pi i-\frac{4}{3}\pi\cot\frac{\pi}{h}z+\frac{1}{3}\pi\cot\frac{\pi}{2h}z & ; \quad \text{Im } z < 0 \end{cases}, \tag{4.2}$$

which can be approximated as

$$|\Phi_s(z)| \simeq \frac{2}{3}\pi\exp(-\pi|y|/h) \quad , \quad |\mathrm{Im}\ z| \gg h \quad . \tag{4.3}$$

Comparing this with (3.1) we see that the decay rate of the exponent of (4.3) is half of that of (3.1). We see this situation also from the point of (3.9). Indeed, if we put $\Phi_s(z)=0$ in (4.2) for Im $z>0$, we find an infinite array of zeros of $\Phi_s(z)$ in the upper half-plane arranged with distance of $2h=2(b-a)/n$ at

$$z = i\frac{h}{\pi}\log 3 + 2jh \quad , \ j=0,\pm1,\pm2,\dots \quad . \tag{4.4}$$

This means $n_z=n/2$, and hence the asymptotic decay rate for Simpson's formula is

$$r = \frac{\pi n}{b-a} = \frac{\pi}{h} \tag{4.5}$$

from (3.9).

It should be remarked that there may happen to be a case where an approximate formula other than the trapezoidal rule gives better result for certain analytic periodic functions. In fact Simpson's formula (4.1) would yield an exact result except the round-off error when applied to a meromorphic function having simple poles the location of which coincides with that of zeros (4.4) of $\Phi_s(z)$. Such a case, however, is rather exceptional and , since the asymptotic approximation of $|\Phi_n(z)|$ such as (3.1) or (4.3) becomes more precise as h is made smaller, the trapezoidal rule would become superior to any other formulas when a high precision is required so that the number of the sampling points is sufficiently large.

Finally we show a numerical example that shows the superiority of the trapezoidal rule. To the integral representation of Bessel function

$$J_4(5) = \frac{I}{\pi} \int_0^{\pi} \cos(4x-5\sin x)dx \tag{4.6}$$

we applied the trapezoidal rule, Simpson's formula, Filon's formula [2] and Legendre-Gauss rule. The number of the sampling points of each formula is chosen to be 16. The computed absolute errors are as follows:

Integration formula	Absolute error
Trapezoidal rule	3.7×10^{-19}
Simpson's formula	2.5×10^{-5}
Filon's formula	2.4×10^{-3}
Legendre-Gauss rule	6.1×10^{-8} .

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Numerical Investigation of 1/2-Subharmonic Solutions to Duffing's Equation

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1. Introduction

The present paper is concerned with 1/2-subharmonic solutions to Duffing's equation

$$(1.1) \qquad \frac{d^2x}{dt^2} + a\cdot\frac{dx}{dt} + bx + cx^3 = e\cdot\cos\omega t,$$

where $b>0$, $c>0$ and $e>0$.

The mathematical proof for the existence of a 1/2-subharmonic solution to (1.1) with damping absent, that is, with $a=0$, has been given by C.T. Taam [6], T. Shimizu [3] and W.S. Loud [2]. But, as far as the author is aware, good approximations to 1/2-subharmonic solutions are not yet found and the mathematical proof for the existence of a 1/2-subharmonic solution is not yet given to Duffing's equation (1.1) with damping present, that is, with $a\neq 0$.

In the present paper, good Galerkin approximations to the subharmonic solutions in question will be given by means of Galerkin's procedure established by M. Urabe [7] and of the author's program [5] of finding solutions to systems of non-linear equations, and the mathematical guarantee for the existence of the corresponding exact subharmonic solutions will be also given by the use of Urabe's existence theorem [7].

Replacing ωt by t, we rewrite (1.1) as follows:

$$(1.2) \qquad \frac{d^2x}{dt^2} + \frac{a}{\omega}\cdot\frac{dx}{dt} + \frac{1}{\omega^2}\cdot(bx+cx^3) = \frac{e}{\omega^2}\cos t.$$

To a 1/2-subharmonic solution to (1.1), corresponds a solution to (1.2) of the form

(1.3) $$x(t)=c_1+\sum_{n=1}^{\infty}(c_{2n}\cdot \sin\frac{n}{2}t + c_{2n+1}\cdot \cos\frac{n}{2}t).$$

Hence, replacing t by 2t in (1.2) and (1.3), we can reduce the problem to the one to find a solution of the form

(1.4) $$x(t)=c_1+\sum_{n=1}^{\infty}(c_{2n}\cdot \sin nt + c_{2n+1}\cdot \cos nt)$$

to the equation

(1.5) $$\frac{d^2x}{d\ t^2} + \alpha\cdot\frac{dx}{dt} + \beta x + \gamma x^3 = P\cdot \cos 2t,$$

where

$$\alpha=\frac{2}{\omega}a,\quad \beta=(\frac{2}{\omega})^2 b,\quad \gamma=(\frac{2}{\omega})^2 c,\quad P=(\frac{2}{\omega})^2 e.$$

The equation (1.5) can be rewritten in the following form

(1.6) $$\frac{d^2y}{d\ t^2} + \alpha\cdot\frac{dy}{dt} + \beta y + y^3 = P\sqrt{\gamma}\cos 2t,$$

where $y=\sqrt{\gamma}x$. The equation (1.5) can be also rewritten in a standard form as follows:

(1.7) $$\frac{d^2z}{d\ \tau^2} + \sigma\cdot\frac{dz}{d\tau} + z + \varepsilon\cdot z^3 = \cos\ \nu\tau\ ,$$

where

$$\sqrt{\beta}\cdot t=\tau\ ,\quad \frac{\beta}{P}x=z,\quad \frac{\alpha}{\sqrt{\beta}}=\sigma\ ,\quad \frac{\gamma\cdot P^2}{\beta^3}=\varepsilon\ ,\quad \frac{2}{\sqrt{\beta}}=\nu\ .$$

As for 1/2-subharmonic solutions to (1.5) with damping present, C. Hayashi [1] suggests some interesting properties from his phase-plane analysis, but his assertions are made from rough approximate solutions of the form

$$x(t)=c_1+c_2\cdot \sin t + c_3\cdot \cos t - \frac{P}{3}\cdot \cos 2t$$

without giving the proof for the existence of 1/2-subharmonic solutions. Hence, his assertions do not seem to be of enough mathematical confidence.

In the present paper, at first, we compute Galerkin approximate solutions of the form

$$x(t)=c_1+c_2\cdot\sin t+c_3\cdot\cos t+c_4\cdot\sin 2t+c_5\cdot\cos 2t$$

by the use of the author's geometric method [4],[5] and then , starting from these rough approximate solutions, we compute the approximations to the solutions of the form (1.4) by the use of Galerkin's procedure established by M. Urabe [8].

After having found an approximate solution by the above procedure, it is necessary for the completion of the process to verify the existence of an exact solution near the approximate solution obtained and to find an error bound for the approximate solution obtained. Using the method developed by M. Urabe [7] , we have checked the existence of the exact subharmonic solutions and we have calculated the error bounds for the approximate solutions. In Tables 2~8, δ shows the error bound obtained in this way. In Tables 1~9, the stability of the subharmonic solutions are also shown.

The computations in the present paper have been carried out by the use of TOSBAC 3400 at the Computing Institution of the Reseach Institute for Mathematical Sciences, Kyoto University.

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2. Numerical Computation

In his paper [8], M. Urabe established a Galerkin procedure to compute numerically the solutions of the form (1.4) to the equation (1.5) by solving the so-called determining equation by the Newton method. In the present paper, we shall use his procedure. According to Urabe's procedure, we rewrite equation (1.5) in the first order system

$$(2.1)\qquad \begin{cases} \dot{x}=y, \\ \dot{y}=X(x,y,t) \end{cases} \qquad (\cdot=d/dt)$$

where $X(x,y,t)=-\beta x-\gamma x^3-\alpha y+P\cdot\cos 2t$.
For (2.1), a Galerkin approximation of order m is of the form

$$(2.2)\qquad \begin{cases} \bar{x}(t)=c_1+\sum_{n=1}^{m}(c_{2n}\cdot\sin nt+c_{2n+1}\cdot\cos nt), \\ \bar{y}(t)=\sum_{n=1}^{m}(-n\cdot c_{2n+1}\cdot\sin nt+n\cdot c_{2n}\cdot\cos nt). \end{cases}$$

Hence, for (2.2), the determining equation for the Galerkin approximations of order m can be reduced to the following equation

$$(2.3)\qquad \begin{cases} f_1(C)=\frac{1}{2\pi}\int_0^{2\pi} X[\bar{x}(t),\bar{y}(t),t]\,dt=0, \\ f_{2n}(C)=\frac{1}{\pi}\int_0^{2\pi} X[\bar{x}(t),\bar{y}(t),t]\cdot\sin nt\,dt+n^2\cdot c_{2n}=0, \\ f_{2n+1}(C)=\frac{1}{\pi}\int_0^{2\pi} X[\bar{x}(t),\bar{y}(t),t]\cdot\cos nt\,dt+n^2\cdot c_{2n+1}=0 \end{cases}$$

$$(n=1,2,\ ---\ ,m),$$

where $C=(c_1,c_2,\ ---\ ,c_{2m},c_{2m+1})$.

In order to apply the Newton method to the system (2.3), it is necessary to find the starting approximate solutions to the determining equations (2.3). For this purpose we consider a Galerkin approximation (2.2) with m=2, that is,

(2.4) $\bar{x}(t)=c_1+c_2\cdot\sin t+c_3\cdot\cos t+c_4\cdot\sin 2t+c_5\cdot\cos 2t.$

Then the determining equations for (2.4) are as follows:

$$(2.5)\quad\begin{cases} f_1(c_1,c_2,c_3,c_4,c_5)=\beta c_1+\gamma(c_1^3+1.5c_1c_2^2+0.75c_3^2c_5+1.5c_1c_3^2 \\ \quad +1.5c_1c_4^2+1.5c_1c_5^2+1.5c_2c_3c_4-0.75c_2^2c_5)=0, \\ f_2(c_1,c_2,c_3,c_4,c_5)=(\beta-1)c_2-\alpha c_3+\gamma(0.75c_2^3+3c_1^2c_2 \\ \quad +0.75c_2c_3^2+1.5c_2c_4^2+1.5c_2c_5^2-3c_1c_2c_5+3c_1c_3c_4)=0, \\ f_3(c_1,c_2,c_3,c_4,c_5)=\alpha c_2+(\beta-1)c_3+\gamma(0.75c_3^3+3c_1^2c_3 \\ \quad +0.75c_2^2c_3+1.5c_3c_4^2+1.5c_3c_5^2+3c_1c_2c_4+3c_1c_3c_5)=0, \\ f_4(c_1,c_2,c_3,c_4,c_5)=(\beta-4)c_4-2\alpha c_5+\gamma(0.75c_4^3+3c_1^2c_4 \\ \quad +1.5c_2^2c_4+1.5c_3^2c_4+0.75c_4c_5^2+3c_1c_2c_3)=0, \\ f_5(c_1,c_2,c_3,c_4,c_5)=2\alpha c_4+(\beta-4)c_5-P+\gamma(0.75c_5^3+3c_1^2c_5 \\ \quad +1.5c_2^2c_5-1.5c_1c_2^2+1.5c_3^2c_5+1.5c_1c_3^2+0.75c_4^2c_5)=0. \end{cases}$$

For a system of the above determining equations with
$\alpha=0.1$, $\beta=0.3$, $\gamma=0.7$, $P=2.0$
that is,
$\sigma=0.183$, $\varepsilon=103.704$, $\nu=3.651$,
we have computed the eleven solutions shown in Table 1 in the bounded region $|c_i|\leqq 3$ $(i=1,2,3,4,5)$, by the use of the fortran program constructed in the previous paper [5].

Now from the form of (1.5), we can easily see that if x(t) is a solution to (1.5), then $x(t+\pi)$, $-x[t+(3\pi/2)]$ and $-x[t+(\pi/2)]$ are also solutions to (1.5), and that if $\bar{x}(t)$ is a Galerkin approximation of 2π-periodic solution to (1.5), then $\bar{x}(t+\pi)$, $-\bar{x}[t+(3\pi/2)]$ and $-\bar{x}[t+(\pi/2)]$ are also Galerkin approximations of 2π-periodic solutions to (1.5) with the same order as $\bar{x}(t)$.

For the solutions to (2.5) shown in Table 1, we readily see that the Galerkin approximations $\bar{x}_2(t)$, $\bar{x}_5(t)$ and $\bar{x}_6(t)$ corresponding to the 2nd, 5th and 6th solutions in Table 1 are equal respectively to $\bar{x}_1(t+\pi)$, $-\bar{x}_1[t+(3\pi/2)]$ and $-\bar{x}_1[t+(\pi/2)]$, where $\bar{x}_1(t)$ is the Galerkin approximation corresponding to the first solution in Table 1.
Likewise we readily see that the Galerkin approximations $\bar{x}_4(t)$, $\bar{x}_7(t)$ and $\bar{x}_8(t)$ corresponding to the 4th, 7th and 8th solutions in Table 1 are equal respectively to $\bar{x}_3(t+\pi)$, $-\bar{x}_3[t+(3\pi/2)]$ and $-\bar{x}_3[t+(\pi/2)]$, where $\bar{x}_3(t)$ is the Galerkin approximation corresponding to the 3rd solution in Table 1.

The Galerkin approximations $\bar{x}_9(t)$, $\bar{x}_{10}(t)$ and $\bar{x}_{11}(t)$ corresponding to the 9th, 10th and 11th solutions in Table 1 will be supposed to be the Galerkin approximations of harmonic solutions to (1.2).

Starting from the solutions to (2.5) shown in Table 1, by the use of the techniques described in the paper [8] we have computed the Galerkin approximations of high order for subharmonic solutions and harmonic solutions. However, by the reason mentioned above, we have not carried out the computations starting from the 2nd, 4th, 5th, 6th, 7th and 8th solutions in Table 1. The results are shown in Tables 2 and 3. In these tables, for each approximate solution is given an error bound δ such that

$$[|\bar{x}(t) - \hat{x}(t)|^2 + |\dot{\bar{x}}(t) - \dot{\hat{x}}(t)|^2]^{\frac{1}{2}} \leq \delta,$$

where $\cdot = d/dt$ and $\hat{x}(t)$ is an exact solution corresponding to the approximate solution $\overline{x}(t)$.

3. The Effect of Nonlinear Term on the Subharmonic Solutions

In order to consider the subharmonic solutions to weakly nonlinear equation (1.5), that is, equation (1.5) with $|\gamma| \ll 1$, we pursue a behavior of the stable subharmonic solution $\overline{x}_3(t)$ obtained in the previous section as $\gamma \longrightarrow 0$.

From the last equation of (2.5) we have

$$1.5\,\gamma c_2^2(c_5-c_1)+1.5\gamma\, c_3^2(c_5+c_1)=P-2\,\alpha c_4+(4-\beta)c_5-\gamma c_5(0.75\,c_5^2+3c_1^2+0.75c_4^2).$$

Taking account of the numerical results, we may consider that the value of c_5 is close to $-P/3$ which does not vanish for $P=2.0$. Hence, we have

$$\left(1-\frac{c_1}{c_5}\right) c_2^2 + \left(1+\frac{c_1}{c_5}\right) c_3^2 = \frac{2P-4\alpha c_4+(8-2\beta)c_5}{3\gamma c_5} - \frac{1.5c_5^2+6c_1^2+1.5c_4^2}{3}.$$

Letting $\alpha \to 0$ and $\gamma \to 0$, we see from the results of the numerical computations that $|c_1/c_5|<1$ and $|c_4| \ll 1$.
Hence, for small values of γ and $|\alpha|$, we may estimate the amplitude $\sqrt{c_2^2+c_3^2}$ of the principal part of 1/2-subharmonic solution as follows:

$$\text{(3.1)} \qquad \sqrt{c_2^2+c_3^2} \approx \left[\frac{2P+(8-2\beta)c_5}{3\,\gamma c_5}\right]^{\frac{1}{2}}.$$

The value of the right side of (3.1) tends to infinity as γ approaches zero. Hence, the amplitude of the subharmonic solution increases as the value of γ decreases.

Fig. 2 shows this phenomenon by waveforms of the stable subharmonic solution $\overline{x_3}(t)$ for various values of γ .
These solutions are shown in Tables 4 ~ 6.
These results show that 1/2-subharmonic solutions to Duffing's equation do not exist in a neighborhood of periodic solutions to the linearized equation. The fact tells us that the methods of perturbation which seek for solutions in a neighborhood of solutions to the linearized equation are not adequate for the computation of 1/2-subharmonic solutions to Duffing's equation. This may be the main reason why 1/2-subharmonic solutions to Duffing's equation have been never computed so far.

M. Urabe [9] proves that for sufficiently small values of ε and $\sigma(>0)$ there exists only the 1/3-subharmonic solution to (1.7), except for the solutions z(t) such that $|z(t)| \to \infty$ or $|dz/dt| \to \infty$ as $\varepsilon \to 0$.
Our results illustrate affirmatively his result.

From (3.1) the amplitude $\sqrt{c_2^2 + c_3^2}$ of the principal part of 1/2-subharmonic solutions tends to infinity with order $\gamma^{-\frac{1}{2}}$ as γ approaches zero. But the value of $\sqrt{\gamma} \cdot \sqrt{c_2^2 + c_3^2}$ is nearly constant as γ approaches zero. The fact tells us that it is better to compute 1/2-subharmonic solutions to (1.6) instead of (1.5) for small values of α and γ .
Taking account of the fact, we have computed the subharmonic solutions to (1.6) with α=0.00001, β=0.3, γ=0.0000675 and P=2.0. The results are shown in Table 9.

Tables 2 ~ 9 show that in the Fourier series of the subharmonic solution in question, the first five terms dominate the remaining ones in strongly nonlinear cases, but the first seven terms dominate the remaining ones in weakly nonlinear cases. The fact tells us that one can know the qualitative character of 1/2-subharmonic solutions to strongly nonlinear Duffing's equation by investigating the character of the Galerkin approximations of the form

$$\overline{x}(t)=c_1+c_2\cdot\sin t+c_3\cdot\cos t+c_4\cdot\sin 2t+c_5\cdot\cos 2t,$$

but in weakly nonlinear cases one must take the more accurate Galerkin approximations for the same purpose.

Remark. The effect of the damping term in the stable 1/2-subharmonic solution $\overline{x}_3(t)$ of the form

$$\overline{x}_3(t)=c_1+\sum_{n=1}^{\infty}c_{2n}\cdot\sin nt+\sum_{n=1}^{\infty}c_{2n+1}\cdot\cos nt$$

appears strongly in the terms $\sum_{n=1}^{\infty}c_{2n}\cdot\sin nt$.
When the damping is absent, we observe in Tables 7 and 8 that

$$\sum_{n=1}^{\infty}c_{2n}\cdot\sin nt\ \fallingdotseq 0,$$

but when the damping is present, we observe in Tables 4 and 6 that

$$\sum_{n=1}^{\infty}c_{2n}\cdot\sin nt$$

is not small and it increases as the value of γ decreases.
In this case, however,

$$\sum_{n=1}^{\infty}c_{2n+1}\cdot\cos nt$$

is effected very little by the damping term.

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	c_1	c_2	c_3	c_4
1:	0.0923726693	-0.2752659728	-0.6784945626	0.0597774582
2:	0.0923726692	0.2752659730	0.6784945625	0.0597774582
3:	0.1285965000	-0.1825706906	-0.7583156503	0.0632102469
4:	0.1285964999	0.1825706907	0.7583156503	0.0632102469
5:	-0.0923726692	0.6784945625	-0.2752659730	0.0597774582
6:	-0.0923726693	-0.6784945626	0.2752659728	0.0597774582
7:	-0.1285965000	0.7583156505	-0.1825706905	0.0632102469
8:	-0.1285964999	-0.7583156502	0.1825706909	0.0632102469
9:	0.0000000000	0.0000000000	0.0000000000	0.0319575661
10:	0.0000000000	0.0000000000	0.0000000000	0.8312796602
11:	0.0000000000	0.0000000000	0.0000000000	0.5462865832

	c_5
1:	-0.6783580768
2:	-0.6783580768
3:	-0.6899371440
4:	-0.6899371440
5:	-0.6783580768
6:	-0.6783580768
7:	-0.6899371441
8:	-0.6899371440
9:	-0.5644062145
10:	2.760755463
11:	-2.272539725

Table 1

Periodic solutions to (1.5) with $\alpha=0.1, \beta=0.3, \gamma=0.7, P=2.0$:

1)
$$\begin{aligned}
\overline{x}_1(t)=0.0928604913 &-0.2729725113 \sin t &&-0.6622053451 \cos t \\
&+0.0592095043 \sin 2t &&-0.6775492475 \cos 2t \\
&+0.0081759893 \sin 3t &&-0.0104856750 \cos 3t \\
&-0.0081146901 \sin 4t &&-0.0070125277 \cos 4t \\
&-0.0015293305 \sin 5t &&-0.0075428283 \cos 5t \\
&+0.0005026926 \sin 6t &&-0.0017641013 \cos 6t \\
&-0.0000735301 \sin 7t &&-0.0001068038 \cos 7t \\
&-0.0000611871 \sin 8t &&-0.0000950798 \cos 8t \\
&-0.0000011729 \sin 9t &&-0.0000382199 \cos 9t \\
&+0.0000008986 \sin 10t &&-0.0000054232 \cos 10t \\
&-0.0000010457 \sin 11t &&-0.0000011578 \cos 11t \\
&-0.0000002502 \sin 12t &&-0.0000006431 \cos 12t \\
&+0.0000000026 \sin 13t &&-0.0000001539 \cos 13t \\
&-0.0000000098 \sin 14t &&-0.0000000231 \cos 14t \\
&-0.0000000066 \sin 15t &&-0.0000000092 \cos 15t \\
&-0.0000000009 \sin 16t &&-0.0000000033 \cos 16t \\
&-0.0000000001 \sin 17t &&-0.0000000006 \cos 17t \\
&-0.0000000001 \sin 18t &&-0.0000000001 \cos 18t \\
& &&-0.0000000001 \cos 19t,
\end{aligned}$$

$\delta=1.4\times10^{-7}$, Stability: unstable.

2)
$$\begin{aligned}
\overline{x}_3(t)=0.1325574730 &-0.1765810119 \sin t &&-0.7455563965 \cos t \\
&+0.0627505778 \sin 2t &&-0.6894792968 \cos 2t \\
&+0.0065184359 \sin 3t &&-0.0122670665 \cos 3t \\
&-0.0057077000 \sin 4t &&-0.0096779756 \cos 4t \\
&-0.0002877279 \sin 5t &&-0.0085009813 \cos 5t \\
&+0.0005555277 \sin 6t &&-0.0019074934 \cos 6t \\
&-0.0000489424 \sin 7t &&-0.0001903122 \cos 7t \\
&-0.0000306596 \sin 8t &&-0.0001267016 \cos 8t \\
&+0.0000061376 \sin 9t &&-0.0000442724 \cos 9t \\
&+0.0000015217 \sin 10t &&-0.0000075120 \cos 10t \\
&-0.0000005539 \sin 11t &&-0.0000020591 \cos 11t \\
&-0.0000000308 \sin 12t &&-0.0000008552 \cos 12t \\
&+0.0000000388 \sin 13t &&-0.0000002050 \cos 13t \\
&-0.0000000016 \sin 14t &&-0.0000000445 \cos 14t \\
&-0.0000000021 \sin 15t &&-0.0000000156 \cos 15t \\
&+0.0000000004 \sin 16t &&-0.0000000047 \cos 16t \\
&+0.0000000001 \sin 17t &&-0.0000000011 \cos 17t \\
& &&-0.0000000003 \cos 18t \\
& &&-0.0000000001 \cos 19t,
\end{aligned}$$

$\delta=1.8\times10^{-7}$, Stability: stable.

Table 2

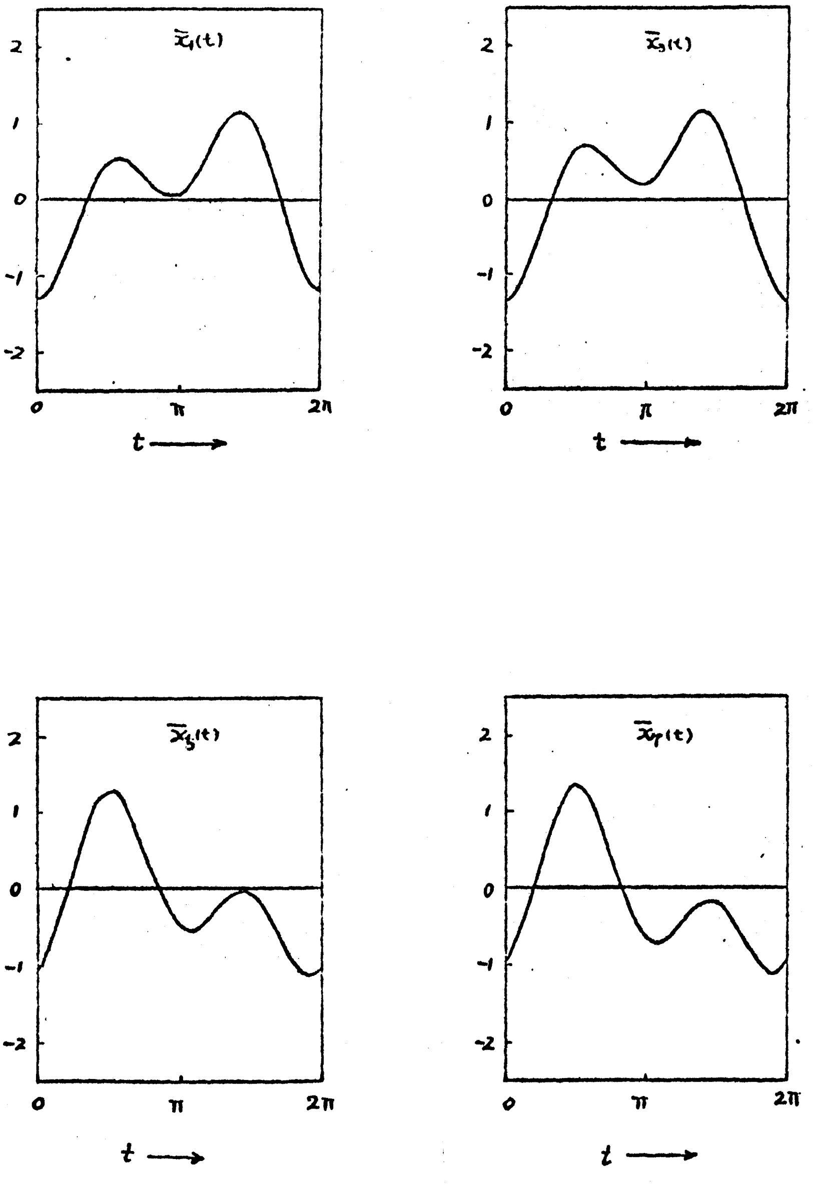

Fig. 1 Waveforms of the 1/2-subharmonic solutions given in Table 2.

Periodic solutions to (1.2) with $\alpha = 0.1$ $\beta = 0.3$, $\gamma = 0.7$, $P = 2.0$:

1) $$\begin{aligned}\bar{x}_9(t) = 0.0000000001 &+ 0.0319635845 \sin t - 0.5644528144 \cos t \\ &+ 0.0001659289 \sin 3t - 0.0008785586 \cos 3t \\ &+ 0.0000004612 \sin 5t - 0.0000014402 \cos 5t \\ &+ 0.0000000011 \sin 7t - 0.0000000023 \cos 7t,\end{aligned}$$

$\delta = 4.7 \times 10^{-9}$, Stability: stable.

2) $$\begin{aligned}\bar{x}_{10}(t) = 0.0000000002 &+ 0.8085998729 \sin t + 2.6920234635 \cos t \\ &+ 0.1077254917 \sin 3t + 0.0940200536 \cos 3t \\ &+ 0.0067635484 \sin 5t + 0.0009948792 \cos 5t \\ &+ 0.0002990601 \sin 7t - 0.0001350083 \cos 7t \\ &+ 0.0000085908 \sin 9t - 0.0000132058 \cos 9t \\ &+ 0.0000000051 \sin 11t - 0.0000007564 \cos 11t \\ &- 0.0000000194 \sin 13t - 0.0000000307 \cos 13t \\ &- 0.0000000016 \sin 15t - 0.0000000007 \cos 15t \\ &- 0.0000000001 \sin 17t,\end{aligned}$$

$\delta = 9.1 \times 10^{-8}$, Stability: stable.

3) $$\begin{aligned}\bar{x}_{11}(t) = 0.0000000001 &+ 0.5305085608 \sin t - 2.2314158468 \cos t \\ &- 0.0000000001 \sin 2t \\ &+ 0.0462811064 \sin 3t - 0.0527460092 \cos 3t \\ &+ 0.0019772093 \sin 5t - 0.0007726566 \cos 5t \\ &+ 0.0000635606 \sin 7t + 0.0000067958 \cos 7t \\ &+ 0.0000016033 \sin 9t + 0.0000010635 \cos 9t \\ &+ 0.0000000281 \sin 11t + 0.0000000506 \cos 11t \\ &+ 0.0000000017 \cos 13t,\end{aligned}$$

$\delta = 3.4 \times 10^{-8}$, Stability: unstable.

Table 3

Periodic solutions to (1.5) with $\alpha=0.001$, $\beta=0.3$, $P=2.0$:

$$
\begin{aligned}
\overline{x}_3(t)=0.2930123755&-1.2590140124\sin t-11.4799570291\cos t\\
&+0.0341190409\sin 2t-0.6997695126\cos 2t\\
&-0.1130152934\sin 3t-0.3336762141\cos 3t\\
&-0.0052523794\sin 4t-0.0329736966\cos 4t\\
&-0.0054219996\sin 5t-0.0101881061\cos 5t\\
&-0.0005610178\sin 6t-0.0014392693\cos 6t\\
&-0.0002349807\sin 7t-0.0003180846\cos 7t\\
&-0.0000342579\sin 8t-0.0000535047\cos 8t\\
&-0.0000098891\sin 9t-0.0000100401\cos 9t\\
&-0.0000017126\sin 10t-0.0000018143\cos 10t\\
&-0.0000004099\sin 11t-0.0000003113\cos 11t\\
&-0.0000000771\sin 12t-0.0000000569\cos 12t\\
&-0.0000000167\sin 13t-0.0000000092\cos 13t\\
&-0.0000000033\sin 14t-0.0000000016\cos 14t\\
&-0.0000000007\sin 15t-0.0000000002\cos 15t\\
&-0.0000000001\sin 16t,
\end{aligned}
$$

$\delta=5.6\times10^{-6}$, Stability: stable, where $\gamma=0.00675\times1.0$.

$$
\begin{aligned}
\overline{x}_3(t)=0.2961798507&-0.1083332858\sin t-5.1275197942\cos t\\
&+0.0071156489\sin 2t-0.6962044099\cos 2t\\
&-0.0093081401\sin 3t-0.1496922067\cos 3t\\
&-0.0009722017\sin 4t-0.0322234685\cos 4t\\
&-0.0004426696\sin 5t-0.0070009504\cos 5t\\
&-0.0000999061\sin 6t-0.0015101723\cos 6t\\
&-0.0000260509\sin 7t-0.0003249848\cos 7t\\
&-0.0000063492\sin 8t-0.0000699167\cos 8t\\
&-0.0000015387\sin 9t-0.0000150223\cos 9t\\
&-0.0000003674\sin 10t-0.0000032274\cos 10t\\
&-0.0000000869\sin 11t-0.0000006931\cos 11t\\
&-0.0000000204\sin 12t-0.0000001488\cos 12t\\
&-0.0000000047\sin 13t-0.0000000319\cos 13t\\
&-0.0000000011\sin 14t-0.0000000069\cos 14t\\
&-0.0000000003\sin 15t-0.0000000015\cos 15t\\
&-0.0000000001\sin 16t-0.0000000003\cos 16t\\
&-0.0000000001\cos 17t,
\end{aligned}
$$

$\delta=5.3\times10^{-7}$, Stability: stable, where $\gamma=0.00675\times5.0$.

Table 4

Periodic solutions to (1.5) with $\alpha=0.001, \beta=0.3, P=2.0$:

$$
\begin{aligned}
\bar{x}_3(t)=0.2914436944 &-0.0378554054 \sin t &&-3.5922663954 \cos t\\
&+0.0037432939 \sin 2t &&-0.7002181244 \cos 2t\\
&-0.0030002747 \sin 3t &&-0.0995051261 \cos 3t\\
&-0.0004751640 \sin 4t &&-0.0313425705 \cos 4t\\
&-0.0001337269 \sin 5t &&-0.0065898220 \cos 5t\\
&-0.0000441812 \sin 6t &&-0.0015028645 \cos 6t\\
&-0.0000107546 \sin 7t &&-0.0003512176 \cos 7t\\
&-0.0000028383 \sin 8t &&-0.0000793848 \cos 8t\\
&-0.0000007390 \sin 9t &&-0.0000181357 \cos 9t\\
&-0.0000001854 \sin 10t &&-0.0000041449 \cos 10t\\
&-0.0000000467 \sin 11t &&-0.0000009443 \cos 11t\\
&-0.0000000116 \sin 12t &&-0.0000002154 \cos 12t\\
&-0.0000000029 \sin 13t &&-0.0000000491 \cos 13t\\
&-0.0000000007 \sin 14t &&-0.0000000112 \cos 14t\\
&-0.0000000002 \sin 15t &&-0.0000000026 \cos 15t\\
& &&-0.0000000006 \cos 16t\\
& &&-0.0000000001 \cos 17t,
\end{aligned}
$$

$\delta=2.2\times10^{-7}$, Stability: stable, where $\gamma=0.00675\times10.0$.

$$
\begin{aligned}
\bar{x}_3(t)=0.1729240185 &-0.0013345231 \sin t &&-0.8434488108 \cos t\\
&+0.0006816817 \sin 2t &&-0.7085991147 \cos 2t\\
&+0.0000573890 \sin 3t &&-0.0152417827 \cos 3t\\
&-0.0000449412 \sin 4t &&-0.0121875975 \cos 4t\\
&+0.0000049194 \sin 5t &&-0.0094382956 \cos 5t\\
&+0.0000061983 \sin 6t &&-0.0021498124 \cos 6t\\
&-0.0000002845 \sin 7t &&-0.0002818746 \cos 7t\\
&-0.0000000987 \sin 8t &&-0.0001522820 \cos 8t\\
&+0.0000001164 \sin 9t &&-0.0000520669 \cos 9t\\
&+0.0000000236 \sin 10t &&-0.0000105388 \cos 10t\\
&-0.0000000010 \sin 11t &&-0.0000028904 \cos 11t\\
&+0.0000000014 \sin 12t &&-0.0000010626 \cos 12t\\
&+0.0000000008 \sin 13t &&-0.0000002833 \cos 13t\\
&+0.0000000001 \sin 14t &&-0.0000000699 \cos 14t\\
& &&-0.0000000218 \cos 15t\\
& &&-0.0000000066 \cos 16t\\
& &&-0.0000000017 \cos 17t\\
& &&-0.0000000005 \cos 18t\\
& &&-0.0000000001 \cos 19t,
\end{aligned}
$$

$\delta=7.0\times10^{-8}$, Stability: stable, where $\gamma=0.00675\times100.0$.

Table 5

Periodic solutions to (1.5) with $\alpha=0.001, \beta=0.3, P=2.0$:

$$
\begin{aligned}
\bar{x}_3(t)=0.1113354509&-0.0010744200 \sin t &&-0.5514182480 \cos t\\
&+0.0005308837 \sin 2t &&-0.6737278095 \cos 2t\\
&+0.0000737828 \sin 3t &&-0.0136047713 \cos 3t\\
&-0.0000344817 \sin 4t &&-0.0055800058 \cos 4t\\
&-0.0000018926 \sin 5t &&-0.0076511441 \cos 5t\\
&+0.0000064399 \sin 6t &&-0.0023812607 \cos 6t\\
&+0.0000002092 \sin 7t &&-0.0001772272 \cos 7t\\
&-0.0000002303 \sin 8t &&-0.0000978628 \cos 8t\\
&+0.0000000720 \sin 9t &&-0.0000496638 \cos 9t\\
&+0.0000000385 \sin 10t &&-0.0000107395 \cos 10t\\
&-0.0000000005 \sin 11t &&-0.0000018419 \cos 11t\\
&-0.0000000001 \sin 12t &&-0.0000008334 \cos 12t\\
&+0.0000000008 \sin 13t &&-0.0000002810 \cos 13t\\
&+0.0000000002 \sin 14t &&-0.0000000598 \cos 14t\\
& &&-0.0000000156 \cos 15t\\
& &&-0.0000000057 \cos 16t\\
& &&-0.0000000016 \cos 17t\\
& &&-0.0000000004 \cos 18t\\
& &&-0.0000000001 \cos 19t,
\end{aligned}
$$

$\delta=7.6\times 10^{-8}$, Stability: stable, where $\gamma=0.00675\times 140.0$.

$$
\begin{aligned}
\bar{x}_3(t)=0.0341643187&-0.0014957675 \sin t &&-0.2491740565 \cos t\\
&+0.0003984503 \sin 2t &&-0.6185496392 \cos 2t\\
&+0.0000860099 \sin 3t &&-0.0092860164 \cos 3t\\
&-0.0000264466 \sin 4t &&-0.0009737959 \cos 4t\\
&-0.0000170626 \sin 5t &&-0.0036648354 \cos 5t\\
&+0.0000047346 \sin 6t &&-0.0021630661 \cos 6t\\
&+0.0000006181 \sin 7t &&-0.0000844859 \cos 7t\\
&-0.0000003103 \sin 8t &&-0.0000226179 \cos 8t\\
&-0.0000000801 \sin 9t &&-0.0000241399 \cos 9t\\
&+0.0000000300 \sin 10t &&-0.0000084863 \cos 10t\\
&+0.0000000020 \sin 11t &&-0.0000005800 \cos 11t\\
&-0.0000000021 \sin 12t &&-0.0000002061 \cos 12t\\
&-0.0000000003 \sin 13t &&-0.0000001293 \cos 13t\\
&+0.0000000002 \sin 14t &&-0.0000000348 \cos 14t\\
& &&-0.0000000037 \cos 15t\\
& &&-0.0000000014 \cos 16t\\
& &&-0.0000000006 \cos 17t\\
& &&-0.0000000002 \cos 18t,
\end{aligned}
$$

$\delta=1.2\times 10^{-7}$, Stability: stable, where $\gamma=0.00675\times 180.0$.

Table 6

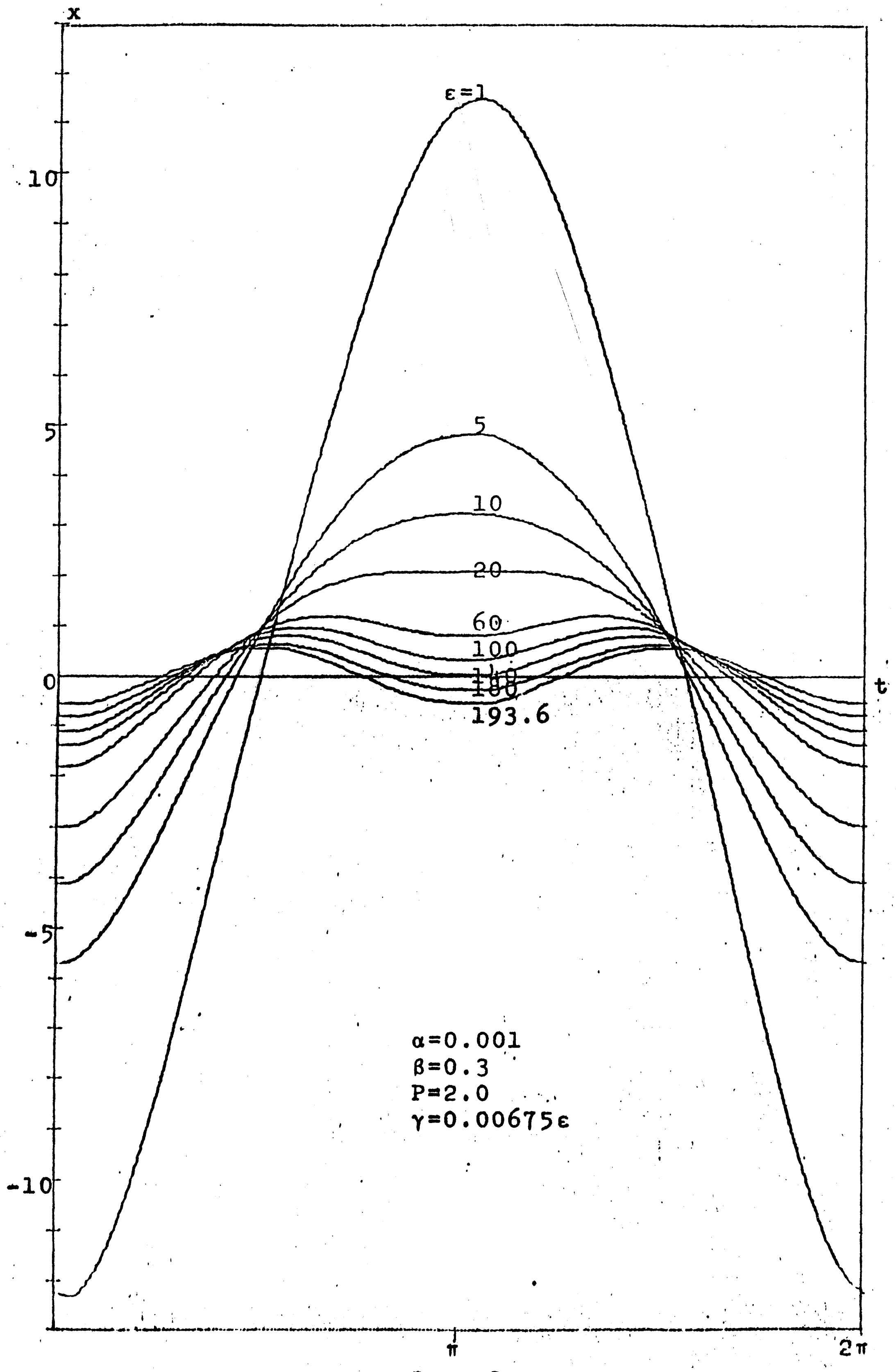
x
10
5
0
-5
-10
t
π
2π
ε=1
5
10
20
60
100
140
180
193.6
α=0.001
β=0.3
P=2.0
γ=0.00675ε

Fig. 2

Periodic solutions to (1.5) with $\alpha=0,\beta=0.3,P=2.0$:

$$
\begin{aligned}
\bar{x}_3(t)=0.3002627613&+0.0000000306\sin t &&-11.5505768414\cos t\\
&-0.0000000011\sin 2t &&-0.6923730347\cos 2t\\
&+0.0000000027\sin 3t &&-0.3526089531\cos 3t\\
&+0.0000000001\sin 4t &&-0.0328902369\cos 4t\\
&+0.0000000001\sin 5t &&-0.0116843449\cos 5t\\
& &&-0.0015252088\cos 6t\\
& &&-0.0004043236\cos 7t\\
& &&-0.0000630335\cos 8t\\
& &&-0.0000144947\cos 9t\\
& &&-0.0000024908\cos 10t\\
& &&-0.0000005309\cos 11t\\
& &&-0.0000000963\cos 12t\\
& &&-0.0000000197\cos 13t\\
& &&-0.0000000037\cos 14t\\
& &&-0.0000000007\cos 15t\\
& &&-0.0000000001\cos 16t,
\end{aligned}
$$

$\delta=5.0\times 10^{-6}$, Stability: neutral, where $\gamma=0.00675\times 1.0$.

$$
\begin{aligned}
\bar{x}_3(t)=0.2964666764&+0.0000000032\sin t &&-5.1288186026\cos t\\
&-0.0000000003\sin 2t &&-0.6959386175\cos 2t\\
&+0.0000000002\sin 3t &&-0.1500079715\cos 3t\\
& &&-0.0322212179\cos 4t\\
& &&-0.0070228217\cos 5t\\
& &&-0.0015132373\cos 6t\\
& &&-0.0003263119\cos 7t\\
& &&-0.0000702336\cos 8t\\
& &&-0.0000151121\cos 9t\\
& &&-0.0000032506\cos 10t\\
& &&-0.0000006991\cos 11t\\
& &&-0.0000001503\cos 12t\\
& &&-0.0000000323\cos 13t\\
& &&-0.0000000070\cos 14t\\
& &&-0.0000000015\cos 15t\\
& &&-0.0000000003\cos 16t\\
& &&-0.0000000001\cos 17t,
\end{aligned}
$$

$\delta=5.1\times 10^{-7}$, Stability: neutral, where $\gamma=0.00675\times 5.0$.

Table 7

Periodic solutions to (1.5) with $\alpha=0, \beta=0.3, P=2.0$:

$$
\begin{aligned}
\bar{x}_3(t)=0.1113376437+0.0000000002 \sin t \; & -0.5514227536 \cos t \\
& -0.6737293984 \cos 2t \\
& -0.0136049668 \cos 3t \\
& -0.0055800896 \cos 4t \\
& -0.0076512213 \cos 5t \\
& -0.0023812868 \cos 6t \\
& -0.0001772325 \cos 7t \\
& -0.0000978644 \cos 8t \\
& -0.0000496646 \cos 9t \\
& -0.0000107398 \cos 10t \\
& -0.0000018420 \cos 11t \\
& -0.0000008334 \cos 12t \\
& -0.0000002811 \cos 13t \\
& -0.0000000598 \cos 14t \\
& -0.0000000156 \cos 15t \\
& -0.0000000057 \cos 16t \\
& -0.0000000016 \cos 17t \\
& -0.0000000004 \cos 18t \\
& -0.0000000001 \cos 19t,
\end{aligned}
$$

$\delta=7.6 \times 10^{-8}$, Stability: neutral, where $\gamma=0.00675 \times 140.0$.

$$
\begin{aligned}
\bar{x}_3(t)=0.0341731575+0.0000000007 \sin t \; & -0.2492037267 \cos t \\
& -0.6185554553 \cos 2t \\
-0.0000000001 \sin 2t \; & -0.0092870763 \cos 3t \\
& -0.0009740593 \cos 4t \\
& -0.0036653121 \cos 5t \\
& -0.0021631498 \cos 6t \\
& -0.0000845008 \cos 7t \\
& -0.0000226241 \cos 8t \\
& -0.0000241435 \cos 9t \\
& -0.0000084870 \cos 10t \\
& -0.0000005801 \cos 11t \\
& -0.0000002062 \cos 12t \\
& -0.0000001294 \cos 13t \\
& -0.0000000348 \cos 14t \\
& -0.0000000037 \cos 15t \\
& -0.0000000014 \cos 16t \\
& -0.0000000006 \cos 17t \\
& -0.0000000002 \cos 18t,
\end{aligned}
$$

$\delta=1.2 \times 10^{-7}$, Stability: neutral, where $\gamma=0.00675 \times 180.0$.

Table 8

Periodic solutions to (1.6) with $\alpha=10^{-5}, \beta=0.3$,
$\gamma=0.00675 \times 10^{-2}, P=2.0$:

$$
\begin{aligned}
\overline{y}_1(t) = \sqrt{\gamma}\cdot\overline{x}_1(t) \\
=0.0005363391 & -0.5948614354 \sin t \quad -0.7414373463 \cos t \\
& +0.0002773728 \sin 2t -0.0069298418 \cos 2t \\
& -0.0263042508 \sin 3t +0.0129549704 \cos 3t \\
& -0.0003350052 \sin 4t -0.0000915269 \cos 4t \\
& +0.0002071635 \sin 5t +0.0008519793 \cos 5t \\
& -0.0000074282 \sin 6t +0.0000141233 \cos 6t \\
& +0.0000261856 \sin 7t -0.0000004987 \cos 7t \\
& +0.0000004872 \sin 8t +0.0000004127 \cos 8t \\
& +0.0000001559 \sin 9t -0.0000007657 \cos 9t \\
& +0.0000000190 \sin 10t -0.0000000144 \cos 10t \\
& -0.0000000212 \sin 11t -0.0000000095 \cos 11t \\
& -0.0000000004 \sin 12t -0.0000000008 \cos 12t \\
& -0.0000000004 \sin 13t +0.0000000006 \cos 13t,
\end{aligned}
$$

Stability: unstable.

$$
\begin{aligned}
\overline{y}_3(t) = \sqrt{\gamma}\cdot\overline{x}_3(t) \\
=0.0024156208 & -0.1036331599 \sin t \quad -0.9449355963 \cos t \\
& +0.0002773708 \sin 2t -0.0057425427 \cos 2t \\
& -0.0094390560 \sin 3t -0.0277658105 \cos 3t \\
& -0.0000433228 \sin 4t -0.0002723404 \cos 4t \\
& -0.0004562977 \sin 5t -0.0007517027 \cos 5t \\
& -0.0000047033 \sin 6t -0.0000118494 \cos 6t \\
& -0.0000182337 \sin 7t -0.0000190670 \cos 7t \\
& -0.0000002870 \sin 8t -0.0000004228 \cos 8t \\
& -0.0000006579 \sin 9t -0.0000004411 \cos 9t \\
& -0.0000000139 \sin 10t -0.0000000131 \cos 10t \\
& -0.0000000221 \sin 11t -0.0000000087 \cos 11t \\
& -0.0000000006 \sin 12t -0.0000000004 \cos 12t \\
& -0.0000000007 \sin 13t -0.0000000001 \cos 13t,
\end{aligned}
$$

Stability: stable.

Table 9

On Numerical Solutions of Stefan Problem I.

Hideo KAWARADA and Makoto NATORI

(Received Jan. 19, 1974; Revised Feb. 15, 1974)

§1. Introduction

Various works have been published on Stefan-type free boundary problems for heat equations.(1)∿(4)

Stefan problem is to seek $u=u(x,t)$ and $s=s(t)$ which satisfy the following equations (FBP.I):

(1.1) $u_t = u_{xx}$, $0<x<s(t)$, $0<t\leqq T$,

(1.2) $u(0,t) = f(t) \geqq 0$, $0\leqq t\leqq T$,

(1.3) $u(s(t),t) = 0$, $0\leqq t\leqq T$,

(1.4) $u(x,0) = \phi(x) \geqq 0$, $0<x\leqq b$, $\phi(b)=0$, $b>0$,

(1.5a) $ds(t)/dt = -u_x(s(t),t)$, $0<t\leqq T$,

(1.5b) $s(0) = b$,

where $0<T<+\infty$. The case $b=0$ will be discussed in the succeeding paper.

The assumption required on the Stefan data is as follows:
Assumption (A): (i) f and ϕ are nonnegative and continuous.
(ii) there exists a positive constant D such that

(1.6) $0 \leqq \phi(x) \leqq D(b-x)$, for $0 \leqq x \leqq b$.

Recently, Nogi(5) presented a difference scheme for FBP.I with a term of artificial heat flow and proved the unique existence and the convergence of the solution of his scheme.

We propose a new difference scheme by the penalty method. Application of the penalty method to initial-boundary value problems in a noncylindrical domain (i.e., moving boundary problems) was done earlier by Fujita.(7)

In order to apply the penalty method to Stefan problems, an integral representation of the free boundary $x=s(t)$ is indispensable.

Therefore, let us use the following reformulation[6] of Stefan condition (1.5):

$$s(t)^2 = F(t) - 2\int_0^{s(t)} \xi u(\xi,t)d\xi \ , \quad 0 \leqq t \leqq T \ , \tag{1.7a}$$

where

$$F(t) = b^2 + 2\int_0^t f(\tau)d\tau + 2\int_0^b \xi\phi(\xi)d\xi \ . \tag{1.7b}$$

We shall denote the differential system (1.1)∿(1.4) and (1.7) by FBP.II.

From (1.7) we see

$$s(t)^2 \leqq F(t) \ , \quad 0 \leqq t \leqq T \ ,$$

since $f(t) \geqq 0$ $(0 \leqq t \leqq T)$ and $u(x,t) \geqq 0$ $(0 \leqq x \leqq s(t), 0 \leqq t \leqq T)$, which follows from maximum principle. Choosing X such that $X \geqq F(t)$, the domain $0<x<s(t)$, $0<t<T$ is included in $\Omega=[0,X]\times[0,T]$. We consider the following equations with the penalty term[7] in the region $\Omega=[0,X]\times[0,T]$,

$$u_t = u_{xx} - K\chi(x,t)u \quad \text{in} \quad \Omega \ , \tag{1.8}$$

$$u(0,t) = f(t) \ , \quad 0 \leqq t \leqq T \ , \tag{1.9}$$

$$u(X,t) = 0 \ , \quad 0 \leqq t \leqq T \ , \tag{1.10}$$

$$u(x,0) = \begin{cases} \phi(x) \ , & 0<x \leqq b \ , \\ 0 \ , & b<x \leqq X \ , \end{cases} \tag{1.11}$$

$$\chi(x,t) = \begin{cases} 0 \ , & 0 \leqq x \leqq s(t), \ 0 \leqq t \leqq T \ , \\ 1 \ , & s(t)<x \leqq X, \ 0 \leqq t \leqq T \ , \end{cases} \tag{1.12}$$

$$s(t)^2 = F(t) - 2\int_0^X \xi u(\xi,t)d\xi \ , \quad 0 \leqq t \leqq T \ , \tag{1.13}$$

where K is a positive number. The system (1.8)∿(1.13) approximates well FBP.II if K is sufficiently large. A merit to solve the above-mentioned system in place of FBP.II is that the calculation is markedly simplified by the replacement of the boundary condition (1.3) on $x=s(t)$ by the boundary condition (1.10) on $x=X$ (which is independent of t).

Now, we introduce the following difference scheme (FBP.III) for the system (1.8)∿(1.13):

$$(1.14)\quad \frac{u_{m,n}-u_{m,n-1}}{k} = \frac{u_{m-1,n-1}-2u_{m,n-1}+u_{m+1,n-1}}{h^2} - K\chi_{m,n}\,u_{m,n}\,,$$

$$1 \leqq m \leqq M-1\ ,\quad 1 \leqq n \leqq N$$

$$(1.15)\quad u_{0,n} = f_n\,,\qquad 0 \leqq n \leqq N$$

$$(1.16)\quad u_{M,n} = 0\,,\qquad 0 \leqq n \leqq N$$

$$(1.17)\quad u_{m,0} = \begin{cases} \phi_m\,, & 1 \leqq m \leqq [b/h] \\ 0\,, & [b/h]+1 \leqq m \leqq M \end{cases}$$

$$(1.18)\quad \chi_{m,n} = \begin{cases} 0\,, & 1 \leqq m \leqq [s_n/h]\,,\ 0 \leqq n \leqq N \\ 1\,, & [s_n/h]+1 \leqq m \leqq M-1\ ,\ 0 \leqq n \leqq N \end{cases}$$

$$(1.19a)\quad s_n^2 = F_n - 2h^2 \sum_{m=1}^{M-1} m\,u_{m,n}\,,\qquad 0 \leqq n \leqq N$$

$$(1.19b)\quad F_n = b^2 + 2k\sum_{n=0}^{n-1} f_n + 2h^2 \sum_{m=1}^{[b/h]} m\phi_m\,.$$

where

h = mesh size in the x direction,

k = mesh size in the t direction,

$T = Nk$,

$X = Mh$,

$u_{m,n} = u(mh,nk)$,

$$s_n = s(nk) ,$$
$$\phi_m = \phi(mh) ,$$
$$f_n = f(nk) ,$$

and $[\alpha]$ denotes the greatest integer not exceeding α .

The objective of the present paper is to construct an approximate solution of FBP.III by iteration.

In the succeeding paper, we will discuss (i) the unique existence of the solution of FBP.III; (ii) the convergence of the solution of FBP.III to the solution of the difference scheme for FBP.II as $K \to \infty$; (iii) the convergence of the difference solution of FBP.II to the solution of the differential system FBP.II as $h, k \to 0$.

In §3, we propose our algorithm. In §4, we show a numerical example. §2 is devoted to the preparation.

§2. Some preliminaries

As a preparation we state the following lemmas.

In FBP.III, the free boundary s_n is determined by (1.19). But if s_n is previously given and K is sufficiently large, we can consider (1.14)∿(1.18) as the system which approximates a moving boundary problem. We shall denote the above-mentioned system by MBP.I. Let the solution of MBP.I be $u^{(K)}_{m,n}$.

Lemma 1. In MBP.I, suppose that $0<k/h^2\leq 1/2$ and that f and ϕ satisfy the assumption (A). Then $u^{(K)}_{m,n}$ satisfies

(2.1) $$0 \leq u^{(K)}_{m,n} \leq C \quad (1\leq m\leq M-1,\ 0\leq n\leq N),$$

where $C = \max\{ \max_{0\leq n\leq N} f_n \,,\ \max_{1\leq m\leq [b/h]} \phi_m\}$.

Proof. From (1.14) we have

(2.2) $$u^{(K)}_{m,n} = \frac{1}{1+kK\chi^{(K)}_{m,n}}\{\lambda u^{(K)}_{m-1.n-1} + (1-2\lambda)u^{(K)}_{m,n-1} + \lambda u^{(K)}_{m+1,n-1}\} ,$$

where

$$\lambda = k/h^2 \quad .$$

By the assumption we see that the coefficients in the braces of the right hand side of (2.2) are all positive and the sum of them equals unity. Making use of the facts

$$0 \leq f_n \leq \max_{0\leq n\leq N} f_n ,$$

and

$$0 \leq \phi_m \leq \max_{1\leq m\leq [b/h]} \phi_m$$

we easily obtain (2.1).

Lemma 2. In MBP.I, let s'_n and s''_n be given and $u'_{m,n}$ and $u''_{m,n}$ be the corresponding solutions. Suppose that $0 \leqq s'_n \leqq s''_n \leqq X$ in $0 \leqq n \leqq N$. Then we have

(2.3) $$u'_{m,n} \leqq u''_{m,n} \quad \text{in} \quad 0 \leqq m \leqq M,\ 0 \leqq n \leqq N.$$

Proof. Put

$$\chi'_{m,n} = \begin{cases} 0 , & 1 \leqq m \leqq [s'_n/h] ,\ 0 \leqq n \leqq N , \\ 1 , & [s'_n/h]+1 \leqq m \leqq M-1,\ 0 \leqq n \leqq N , \end{cases}$$

and

$$\chi''_{m,n} = \begin{cases} 0 , & 1 \leqq m \leqq [s''_n/h] ,\ 0 \leqq n \leqq N , \\ 1 , & [s''_n/h]+1 \leqq m \leqq M-1,\ 0 \leqq n \leqq N . \end{cases}$$

We can prove by induction. First we claim that $u'_{m,1} \leqq u''_{m,1}$. In fact, there holds

$$u'_{m,1} = \frac{1}{1+kK\chi'_{m,1}}\{\lambda u'_{m-1,0} + (1-2\lambda)u'_{m,0} + \lambda u'_{m+1,0}\} \geqq$$

$$\frac{1}{1+kK\ {}''_{m,1}}\{\lambda u''_{m-1,0} + (1-2\lambda)u''_{m,0} + \lambda u''_{m+1,0}\} = u''_{m,1}$$

since $u'_{m,0} = u''_{m,0}$ (initial condition) and $\chi'_{m,1} \geqq \chi''_{m,1}$.

Generally if there holds $u'_{m,n-1} \leqq u''_{m,n-1}$, we get

$$u''_{m,n}-u'_{m,n} = \frac{1}{1+kK\chi''_{m,n}}\{\lambda(u''_{m-1,n-1}-u'_{m-1,n-1})+(1-2\lambda)(u''_{m,n-1}-u'_{m,n-1})$$

$$+ \lambda(u''_{m+1,n-1}-u'_{m+1,n-1})\}+(\frac{1}{1+kK\chi''_{m,n}} - \frac{1}{1+kK\chi'_{m,n}})$$

$$\times\{\lambda u'_{m-1,n-1}+(1-2\lambda)u'_{m,n-1}+\lambda u'_{m+1,n-1}\} \geqq 0 .$$

§3. Algorithm

We shall construct the approximating sequences $\{u_{m,n}^{(\ell)}\}_{\ell=0}^{\infty}$ and $\{s_n^{(\ell)}\}_{\ell=0}^{\infty}$ for FBP.III by the solution of the following difference scheme:

$$(3.1)\quad \frac{u_{m,n}^{(\ell)} - u_{m,n-1}^{(\ell)}}{h} = \frac{u_{m-1,n-1}^{(\ell)} - 2u_{m,n-1}^{(\ell)} + u_{m+1,n-1}^{(\ell)}}{h^2} - K\chi_{m,n}^{(\ell)}u_{m,n}^{(\ell)},$$

$$1 \leqq m \leqq M-1,\ 1 \leqq n \leqq N,$$

$$(3.2)\quad u_{0,n}^{(\ell)} = f_n, \qquad 0 \leqq n \leqq N$$

$$(3.3)\quad u_{M,n}^{(\ell)} = 0, \qquad 0 \leqq n \leqq N$$

$$(3.4)\quad u_{m,0}^{(\ell)} = \begin{cases} \phi_m, & 1 \leqq m \leqq [b/h] \\ 0, & [b/h]+1 \leqq m \leqq M \end{cases}$$

$$(3.5)\quad \chi_{m,n}^{(\ell)} = \begin{cases} 0, & 1 \leqq m \leqq [s_n^{(\ell)}/h],\ 0 \leqq n \leqq N \\ 1, & [s_n^{(\ell)}/h]+1 \leqq m \leqq M-1,\ 0 \leqq n \leqq N \end{cases}$$

$$(3.6a)\quad \{s_n^{(\ell)}\}^2 = F_n - 2h^2 \sum_{m=1}^{M-1} m\, u_{m,n}^{(\ell-1)}, \qquad 0 \leqq n \leqq N,$$

$$(3.6b)\quad \{s_n^{(0)}\}^2 = F_n.$$

The sequences $\{s_n^{(\ell)}\}_{\ell=0}^{\infty}$ and $\{u_{m,n}^{(\ell)}\}_{\ell=0}^{\infty}$ satisfy

$$(3.7)\quad 0 \leqq s_n^{(1)} \leqq s_n^{(3)} \leqq \cdots \leqq s_n^{(2\ell+1)} \leqq \cdots \leqq s_n^{(2\ell)} \leqq \cdots \leqq s_n^{(2)} \leqq s_n^{(0)},$$

$$(3.8)\quad 0 \leqq u_{m,n}^{(1)} \leqq u_{m,n}^{(3)} \leqq \cdots \leqq u_{m,n}^{(2\ell+1)} \leqq \cdots \leqq u_{m,n}^{(2\ell)} \leqq \cdots \leqq u_{m,n}^{(2)} \leqq u_{m,n}^{(0)}.$$

and $s_n^{(\ell)}$ is monotone increasing in n for any ℓ.

This fact can be proved as follows.

First we show $0 \leqq s_n^{(1)}$. Put

$$G_n \equiv \{s_n^{(1)}\}^2 = b^2 + 2k \sum_{n=0}^{n-1} f_n + 2h^2 \sum_{m=1}^{[b/h]} m_m - 2h^2 \sum_{m=1}^{M-1} m\, u_{m,n}^{(0)} .$$

Then we have

$$G_0 = b^2 \geqq 0 .$$

and

$$G_n - G_{n-1} = 2kf_{n-1} - 2h^2 \sum_{m=0}^{M-1} m(u_{m,n}^{(0)} - u_{m,n-1}^{(0)})$$

$$= 2kf_{n-1} - 2k \sum_{m=0}^{M-1} m(u_{m-1,n-1}^{(0)} - 2u_{m,n-1}^{(0)} + u_{m+1,m-1}^{(0)}$$

$$- h^2 K\chi_{m,n}^{(0)}\, u_{m,n}^{(0)})$$

$$= 2k(M-1)u_{M-1,n-1}^{(0)} + 2kh^2 K \sum_{m=0}^{M-1} m\chi_{m,n}^{(0)} u_{m,n}^{(0)} \geqq 0 ,$$

which implies that G_n is monotone increasing in n. Therefore $G_n \geqq 0$ $(0 \leqq n \leqq N)$. Let us set $s^{(1)} = \sqrt{G_n} \geqq 0$.

By Lemma 1 we have

$$\{s_n^{(1)}\}^2 = \{s_n^{(0)}\}^2 - 2h^2 \sum_{m=1}^{M-1} m\, u_{m,n}^{(0)} \leqq \{s_n^{(0)}\}^2 ,$$

from which and Lemma 2 follows $u_{m,n}^{(1)} \leqq u_{m,n}^{(0)}$. Therefore we have

$$\{s_n^{(2)}\}^2 - \{s_n^{(1)}\}^2 = 2h^2 \sum_{m=1}^{M-1} m(u_{m,n}^{(0)} - u_{m,n}^{(1)}) \geqq 0.$$

and

$$\{s_n^{(2)}\}^2 - \{s_n^{(0)}\}^2 = -2h^2 \sum_{m=1}^{M-1} m\, u_{m,n}^{(1)} \leqq 0 ,$$

which implies

$$(3.9) \qquad s_n^{(1)} \leqq s_n^{(2)} \leqq s_n^{(0)} .$$

Using (3.9) and Lemma 2, we have

$$u_{m,n}^{(1)} \leqq u_{m,n}^{(2)} \leqq u_{m,n}^{(0)} \quad .$$

Repeating the similar argument as above, we get (3.7) and (3.8). If we use (3.7) and (3.8), the monotonicity of $s_n^{(\ell)}$ $(\ell \geqq 2)$ in n is shown similarly as $s_n^{(1)}$.

If $|s_n^{(\ell)} - s_n^{(\ell-1)}|$ becomes sufficiently small, $(s_n^{(\ell)}, u_{m,n}^{(\ell)})$ will be considered an approximate solution of FBP.III.

§4. Numerical Example.

We show the result of numerical solution of FBP.III in the case b=1. We choose the following functions as the boundary and initial conditions,

$$f(t) = \begin{cases} \cos\frac{\pi}{4} t \ , & 0 \leqq t \leqq 2 \\ 0 \ , & 2 \leqq t \leqq 2.5 = T \end{cases}$$

$$\phi(x) = 1 - x \ , \qquad 0 \leqq x \leqq 1 \ .$$

In this case, F(t) is calculated by (1.7b) as

$$F(t) = \begin{cases} \frac{4}{3} + \frac{8}{\pi} \sin\frac{\pi}{4} t \ , & 0 \leqq t \leqq 2 \\ \frac{4}{3} + \frac{8}{\pi} \ , & 2 \leqq t \leqq 2.5 \ . \end{cases}$$

Thus we take X equal to 2.5. The coefficient of penalty term K is taken to be 2^{20}. The mesh sizes h and k are

$$h = 1/2^4 \ ,$$

$$k = 1/2^{10} ,$$

The results of calculation are shown in Fig. 1 and 2. After the fifth iteration of (3.6), we get

$$\max_n \left| s_n^{(5)} - s_n^{(6)} \right| = 2.4 \times 10^{-3} \ . \tag{4.1}$$

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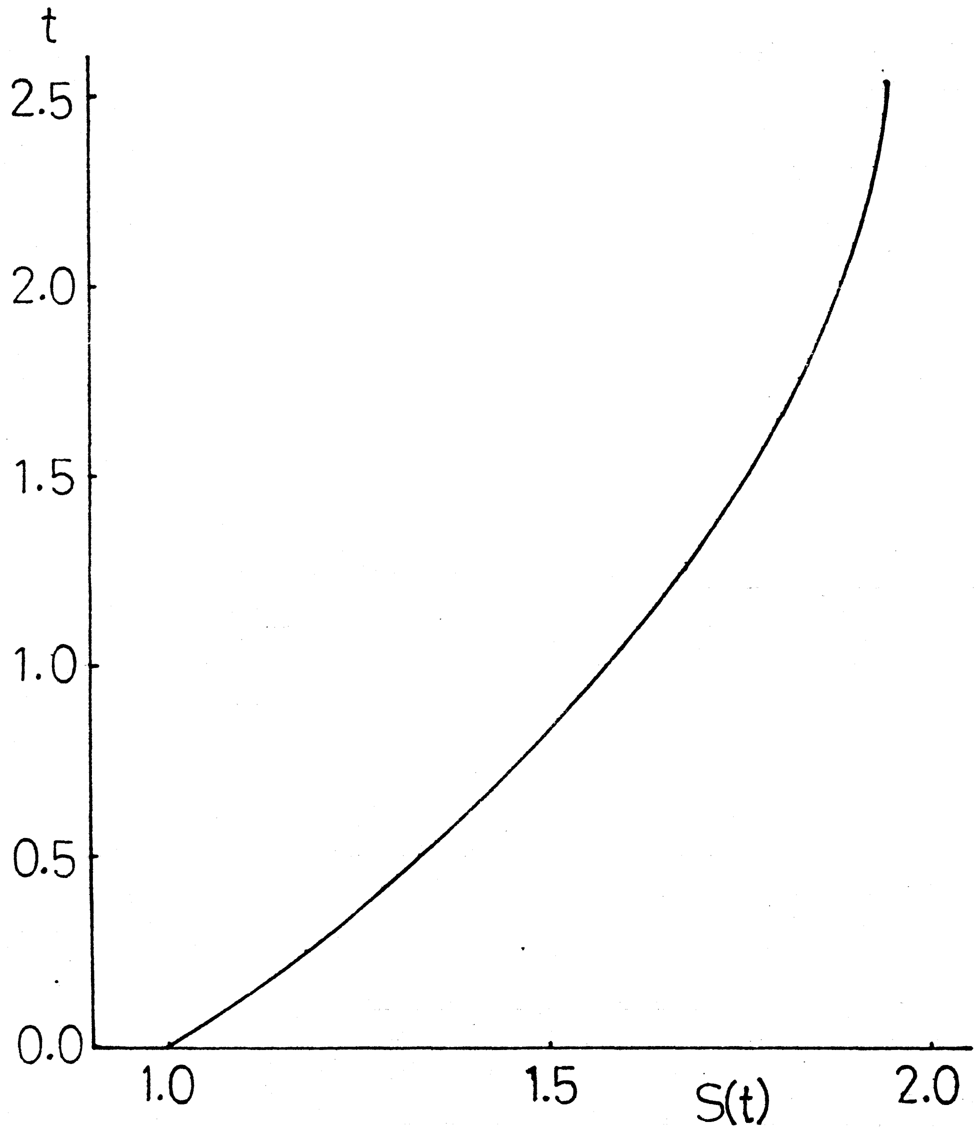
t
2.5
2.0
1.5
1.0
0.5
0.0
1.0
1.5
S(t)
2.0

Fig. 1

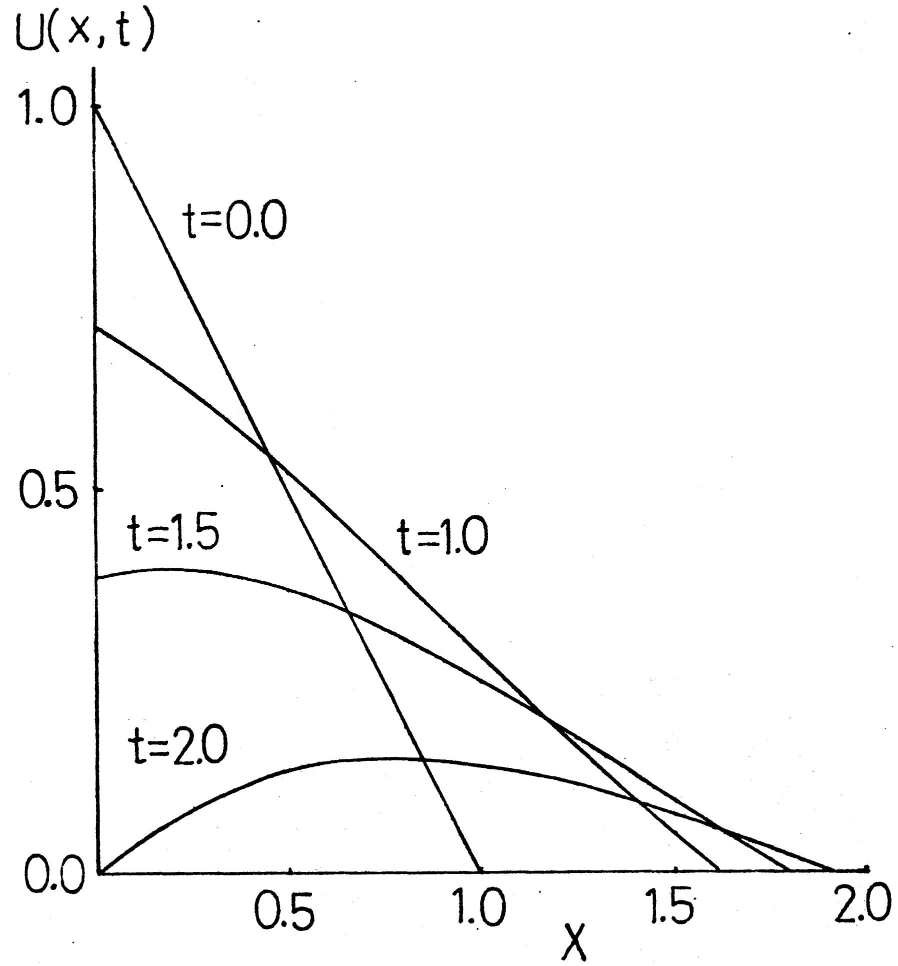
U(x, t)
1.0
0.5
0.0
t=0.0
t=1.0
t=1.5
t=2.0
0.5
1.0
1.5
2.0
X

Fig. 2