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CONVERGENCE OF A SECOND-ORDER SCHEME FOR THE NONLINEAR DYNAMICAL EQUATIONS OF ELASTIC RODS*

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Abstract. A second-order, energy-preserving finite difference scheme to approximate the partial differential equations governing planar, twist-free motions of inextensible, unshearable elastic rods is presented and analyzed.

Key words. energy preserving, second order, dynamics of rods

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1. Introduction. We consider the numerical approximation of the following equations governing the planar motion of a class of inextensible elastic rods:

$$(1.1) \qquad (\cos\theta)_{tt} = f_{ss},$$

$$(1.2) \qquad (\sin\theta)_{tt} = g_{ss},$$

$$(1.3) \qquad \theta_{tt} - \theta_{ss} = -f\sin\theta + g\cos\theta.$$

The unknowns are θ, f, and g, which are each functions of two variables s and t. The system is a generalization of Euler's *elastica* to include inertial dynamics. We assume that the rod is specified by a two-dimensional vector function $\mathbf{r}(s,t) = (x(s,t), y(s,t))$. At time t, $s \mapsto \mathbf{r}(s,t)$ gives the axial curve of the rod in terms of its arc-length parameter s and hence, $|\mathbf{r}_s|^2 = x_s^2 + y_s^2 = 1$. In system (1.1)–(1.3), the variable θ is the angle between the unit tangent $\mathbf{r}_s$ and the x-axis:

$$x_s = \cos\theta, \qquad y_s = \sin\theta.$$

The functions f and g are the stress resultants in the x- and y-directions. They are a priori unknowns, i.e., "reactive forces" similar to the pressure in the theory of incompressible fluid flow. If we assume a linear stress–strain relation, then the dynamical system (1.1)–(1.3) is justified: Equations (1.1) and (1.2) are derived from the balance of linear momentum in the x- and y-directions, and (1.3) is derived from the balance of angular momentum. The three equations are written in dimensionless units.

The system (1.1)–(1.3) was studied by Caflisch and Maddocks [1] in 1984. For finite length rods subject to appropriate boundary conditions, they derived the system (1.1)–(1.3) from a variational principle, proved a global existence theorem, and obtained the dynamical implications of an energy criterion for stability. More recently, Coleman and Dill [2] also derived the system (1.1)–(1.3) from a variational principle, obtained and classified all traveling wave solutions, and raised the question of whether the system is completely integrable.

In this paper, we will present a second-order, energy-preserving scheme to approximate the smooth solution of system (1.1)–(1.3) subject to the boundary conditions

$$(1.4) \qquad \theta(0,t) + 2\pi = \theta(1,t), \quad \theta_s(0,t) = \theta_s(1,t),$$

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(1.5) $f(0,t) = f(1,t), \quad f_s(0,t) = f_s(1,t),$
(1.6) $g(0,t) = g(1,t), \quad g_s(0,t) = g_s(1,t),$

and the initial conditions

(1.7) $\theta(s,0) = \theta_0(s), \qquad \theta_t(s,0) = \theta_1(s).$

The boundary and initial conditions are a simplified version of those boundary and initial conditions used to perform solitary wave scattering experiments. The solitary wave solutions found by Coleman and Dill are defined on $(-\infty, \infty)$ and obey the relations: $\theta \to 0$ as $s \to -\infty$, $\theta \to 2\pi$ or -2π as $s \to \infty$, $f \to \alpha$ as $s \to \pm\infty$, and $\theta_s, f_s, g, g_s \to 0$ as $s \to \pm\infty$, where α is a constant. Since θ, f, and g approach their limits at $\pm\infty$ with an exponential rate, the interactions of solitary waves can be well approximated over a sufficiently large interval L by the boundary and initial conditions given above. Since the analysis does not really depend on the interval length, we have simplified slightly by taking $L = 1$.

We note that many of the ideas for the analysis of the numerical scheme we present here were obtained by finding appropriate discrete versions of the analysis done in [1] for the continuous problem. The design of energy-preserving schemes has a long history, and the energy-preserving property plays an essential role in proving convergence of the schemes; e.g., see [5] and [6], and the references therein.

The scheme has been employed to determine the consequences of the interaction of solitary traveling waves governed by the system (1.1)–(1.3). The numerical results described in Coleman and Xu [3] strongly indicate the system is not completely integrable in the sense of soliton theory. The solitary traveling waves do not interact as solitons; in particular, the change suffered by a solitary wave upon collision with another such wave is more than a shift in phase.

To describe the numerical scheme, we let $\triangle s = h = 1/N$, $(N \in \aleph)$, be the spatial discretization, and $\triangle t = \tau$ be the time step. Denote

$$s_j = jh, \quad t^n = n\tau \qquad (0 \le j \le N, \ n \ge 0),$$
$$\theta_j^n \cong \theta(s_j, t^n), \quad f_j^n \cong f(s_j, t^n), \quad g_j^n \cong g(s_j, t^n).$$

To discretize boundary conditions (1.4)–(1.6), a fictitious point $j = N+1$ is introduced such that

$$\theta_{N+1}^n \cong 2\pi + \theta(s_1, t^n), \quad f_{N+1}^n \cong f(s_1, t^n), \quad g_{N+1}^n \cong g(s_1, t^n).$$

We choose the largest possible time step τ as allowed by the classical Courant–Friedrichs–Lewy (CFL) condition; i.e.,

(1.8) $\tau = h/\sqrt{2}.$

For any mesh function $\{u_j^n\}$, we introduce the operators $\triangle_\tau^2$ and $\triangle_h^2$:

$$\triangle_\tau^2 u_j^n = (u_j^{n+1} - 2u_j^n + u_j^{n-1})/\tau^2,$$
$$\triangle_h^2 u_j^n = (u_{j+1}^n - 2u_j^n + u_{j-1}^n)/h^2.$$

Then the scheme we propose is

(1.9) $\triangle_\tau^2 \cos\theta_j^n = \triangle_h^2 f_j^n,$
(1.10) $\triangle_\tau^2 \sin\theta_j^n = \triangle_h^2 g_j^n,$

$$(1.11) \qquad \triangle_\tau^2 \theta_j^n - \triangle_h^2 \theta_j^n = f_j^n \frac{\cos\theta_j^{n+1} - \cos\theta_j^{n-1}}{\theta_j^{n+1} - \theta_j^{n-1}} + g_j^n \frac{\sin\theta_j^{n+1} - \sin\theta_j^{n-1}}{\theta_j^{n+1} - \theta_j^{n-1}},$$

for $1 \le j \le N$ and $n \ge 1$, subject to the boundary conditions

$$(1.12) \qquad \theta_0^{n+1} + 2\pi = \theta_N^{n+1}, \quad \theta_1^{n+1} + 2\pi = \theta_{N+1}^{n+1},$$

$$(1.13) \qquad f_0^n = f_N^n, \quad f_1^n = f_{N+1}^n,$$

$$(1.14) \qquad g_0^n = g_N^n, \quad g_1^n = g_{N+1}^n,$$

and the initial conditions

$$(1.15) \qquad \theta_j^0 = \varphi_j, \qquad \theta_j^1 = \psi_j.$$

Here $\{\varphi_j\}$ and $\{\psi_j\}$ are mesh functions determined from θ_0 and θ_1 such that

$$(1.16) \qquad \sum_{j=1}^N \cos\psi_j = \sum_{j=1}^N \cos\varphi_j,$$

$$(1.17) \qquad \sum_{j=1}^N \sin\psi_j = \sum_{j=1}^N \sin\varphi_j.$$

The existence of the mesh functions $\{\varphi_j\}$ and $\{\psi_j\}$ will be discussed in §2. The scheme is implicit; more precisely, at each time step $n \ge 1$, we are required to solve a nonlinear algebraic system to find θ_j^{n+1}, f_j^n, g_j^n ($0 \le j \le N+1$). An iterative scheme is presented along with a convergence result for solving this nonlinear system.

The structure of the paper is as follows: In §2, we cite some results for the exact solution $\tilde\theta$, $\tilde f$, and $\tilde g$ and prove the conservation of the discrete energy for the scheme (1.9)–(1.15). In §3, we will rewrite system (1.9)–(1.11) as a second-order semilinear finite difference equation for $\{\theta_j^n\}$. Its right-hand side is nonlocal but does not involve second-order differences; bounds for the right-hand side are presented in §4. Results on solvability are presented in §5, and an error estimate is derived in §6.

We conclude this section by introducing some notation. Given a mesh function u_j^n, $1 \le j \le N$, $n \ge 0$, we write $u_h^n = (u_1^n, u_2^n, \ldots, u_N^n)^T$, $\triangle_\tau^+ u_j^n = (u_j^{n+1} - u_j^n)/\tau$,

$$(1.18) \qquad \tilde D_h^- u_j^n = \begin{cases} (u_1^n - u_N^n)/h & \text{if } j = 1, \\ (u_j^n - u_{j-1}^n)/h & \text{if } 2 \le j \le N; \end{cases}$$

$$(1.19) \qquad D_h^- u_j^n = \begin{cases} (u_1^n - u_N^n + 2\pi)/h & \text{if } j = 1, \\ (u_j^n - u_{j-1}^n)/h & \text{if } 2 \le j \le N; \end{cases}$$

$$(1.20) \qquad D_h^2 u_j^n = \begin{cases} (u_2^n - 2u_1^n + u_N^n - 2\pi)/h^2 & \text{if } j = 1, \\ (u_{j+1}^n - 2u_j^n + u_{j-1}^n)/h^2 & \text{if } 2 \le j \le N-1, \\ (u_{N-1}^n - 2u_N^n + u_1^n + 2\pi)/h^2 & \text{if } j = N. \end{cases}$$

We remark that D_h^- and D_h^2 are the standard backward difference and second-order centered difference, if we introduce the boundary terms $u_0^n = u_N^n - 2\pi$ and $u_{N+1}^n = u_1^n + 2\pi$. However, D_h^- and D_h^2 are helpful when we reformulate the scheme (1.9)–(1.15) in §3, since it is easier to modify the operators than to retain the boundary

conditions. We also define the norms $\|\cdot\|_\infty$, $\|\cdot\|_0$, $\|\cdot\|_e$, and functional $|\cdot|_e$:

$$\|u_h^n\|_\infty = \max_{1\leq j\leq N} |u_j^n|, \quad \|u_h^n\|_0 = \left(h\sum_{j=1}^N (u_j^n)^2\right)^{\frac{1}{2}},$$

$$\|u_h^n\|_e = \left(\|u_h^n\|_0^2 + \|\triangle_\tau^+ u_h^n\|_0^2 + \|\tilde{D}_h^- u_h^n\|_0^2\right)^{\frac{1}{2}}, \quad |u_h^n|_e = \left(\|\triangle_\tau^+ u_h^n\|_0^2 + \|D_h^- u_h^n\|_0^2\right)^{\frac{1}{2}}.$$

Note that $|\cdot|_e$ is not a seminorm for $u_h^n = (u_1^n, u_2^n, \ldots, u_N^n)^T$. However, if we had defined D_h^- as the usual backward difference operator, this quantity would be just a rewriting of a standard seminorm on mesh functions $(u_0^n, u_1^n, u_2^n, \ldots, u_N^n)^T$ for those functions which satisfy the constraint $u_0^n = u_N^n - 2\pi$.

Throughout the paper, C will denote a positive constant, independent of h, τ, and unknown functions, but not necessarily the same at each occurrence.

2. The approximation scheme and the exact solution. We first cite some results about the exact solution $\tilde{\theta}$, $\tilde{f}$, and $\tilde{g}$ [8].

DEFINITION 1. *The class C_{pw}^n is defined to be those functions in C^{n-1} that have piecewise continuous derivatives of order n.*

THEOREM 1. *Let $\theta_0 \in C_{pw}^2([0,1])$ and $\theta_1 \in C_{pw}^1([0,1])$ be given such that*

(2.1) $\qquad \theta_0(0) + 2\pi = \theta_0(1), \qquad \theta_0'(0) = \theta_0'(1), \qquad \theta_1(0) = \theta_1(1),$

(2.2) $\qquad \displaystyle\int_0^1 \theta_1 \sin\theta_0 ds = 0, \qquad \int_0^1 \theta_1 \cos\theta_0 ds = 0.$

Then there exists a unique $\tilde{\theta} \in C_{pw}^2([0,1]\times[0,\infty))$ and $\tilde{f}$, $\tilde{g}$ such that $\tilde{f}_{ss}$, $\tilde{g}_{ss} \in C_{pw}([0,1]\times[0,\infty))$ satisfying equations (1.1)–(1.3) with the boundary conditions (1.4)–(1.6) and initial condition (1.7).

Throughout the paper, we suppose $\theta_0 \in C^4([0,1])$ and $\theta_1 \in C^3([0,1])$ not only satisfy (2.1), (2.2) but also the additional conditions:

(2.3) $\quad \theta_0''(0) = \theta_0''(1), \qquad \theta_0'''(0) = \theta_0'''(1), \qquad \theta_1'(0) = \theta_1'(1), \qquad \theta_1''(0) = \theta_1''(1).$

Since no regularity results are known so far, we *assume* that the exact solution $\tilde{\theta}$, $\tilde{f}$, and $\tilde{g}$ are all in $C^4([0,1]\times[0,T])$ for some $T > 0$.

There are four conserved quantities for the system (1.1)–(1.3) subject to boundary conditions (1.4)–(1.6) (cf. [3], [7]). To express these quantities, let

$$x(s,t) = \int_0^s \cos\theta(\eta,t)d\eta - \int_0^1\int_0^\xi \cos\theta(\eta,t)d\eta d\xi,$$

$$y(s,t) = \int_0^s \sin\theta(\eta,t)d\eta - \int_0^1\int_0^\xi \sin\theta(\eta,t)d\eta d\xi.$$

Then we have the following.

1. *Energy.* $d\mathcal{H}/dt = 0$, where

$$\mathcal{H} = \frac{1}{2}\int_0^1 (\theta_s^2 + \theta_t^2 + x_t^2 + y_t^2)ds.$$

2. *Linear momentum.* $d\mathcal{M}^x/dt = 0$ and $d\mathcal{M}^y/dt = 0$, where

$$\mathcal{M}^x = \int_0^1 x_t ds, \qquad \mathcal{M}^y = \int_0^1 y_t ds.$$

3. *Angular momentum.* $d\mathcal{L}/dt = 0$, where

$$\mathcal{L} = \int_0^1 (\theta_t + xy_t - yx_t)ds$$

$$+ (x(1,t) - x(0,t)) \int_0^t \hat{g}(\tau)d\tau - (y(1,t) - y(0,t)) \int_0^t \hat{f}(\tau)d\tau,$$

in which $\hat{f}(t) = f(0,t) = f(1,t)$ and $\hat{g}(t) = g(0,t) = g(1,t)$.

4. *Linear impulse.* $d\mathcal{I}/dt = 0$, where

$$\mathcal{I} = \int_0^1 (\theta_t\theta_s + x_tx_s + y_ty_s)ds.$$

Our scheme (1.9)–(1.15) preserves the discrete analogues of the first two quantities. To show this, we introduce the mesh functions x_j^n and y_j^n, which are the discrete analogues of x and y. For $1 \le j \le N+1$ and $n \ge 0$,

(2.4) $$x_j^n = -h^2 \sum_{k=1}^{N} \sum_{i=1}^{k-1} \cos\theta_i^n + h \sum_{i=1}^{j-1} \cos\theta_i^n,$$

(2.5) $$y_j^n = -h^2 \sum_{k=1}^{N} \sum_{i=1}^{k-1} \sin\theta_i^n + h \sum_{i=1}^{j-1} \sin\theta_i^n.$$

It is clear from the definition, for $1 \le j \le N$ and $n \ge 0$, we have

(2.6) $$(x_{j+1}^n - x_j^n)/h = \cos\theta_j^n,$$
(2.7) $$(y_{j+1}^n - y_j^n)/h = \sin\theta_j^n.$$

For each $n \ge 1$ fixed, we solve boundary value problem (BVP) (1.9), (1.13) and BVP (1.10), (1.14), respectively, in terms of $\{\theta_j^n\}$. It is not difficult to show that for $1 \le j \le N$, $n \ge 1$,

(2.8) $$\triangle_\tau^2 x_j^n = \triangle_h^- f_j^n,$$
(2.9) $$\triangle_\tau^2 y_j^n = \triangle_h^- g_j^n,$$

where $\triangle_h^-$ is the standard backward difference operator. If we define the discrete linear momentums as

$$M_h^x(n) = h \sum_{j=1}^{N} \triangle_\tau^+ x_j^n, \qquad M_h^y(n) = h \sum_{j=1}^{N} \triangle_\tau^+ y_j^n,$$

then the identities $M_h^x(n+1) = M_h^x(n)$ and $M_h^y(n+1) = M_h^y(n)$ for $n \ge 0$ follow directly from equations (2.8), (2.9), and the boundary conditions (1.13), (1.14).

To find the boundary conditions that x_j^n and y_j^n satisfy, we sum j from 1 to N in equations (1.9) and (1.10). Using the boundary conditions (1.12), (1.13), we find that for $n \ge 1$,

$$\triangle_\tau^2 \left(\sum_{j=1}^{N} \cos\theta_j^n \right) = 0, \qquad \triangle_\tau^2 \left(\sum_{j=1}^{N} \sin\theta_j^n \right) = 0.$$

It follows that for $n \geq 0$,

$$\triangle_\tau^+ \left(\sum_{j=1}^{N} \cos \theta_j^n \right) = \text{const}, \qquad \triangle_\tau^+ \left(\sum_{j=1}^{N} \sin \theta_j^n \right) = \text{const}.$$

However, from equations (1.16) and (1.17), we see that for $n \geq 0$,

$$\triangle_\tau^+ \left(\sum_{j=1}^{N} \cos \theta_j^n \right) = 0, \qquad \triangle_\tau^+ \left(\sum_{j=1}^{N} \sin \theta_j^n \right) = 0.$$

Using these equations and the definitions (2.4), (2.5), we have

(2.10) $$x_{N+1}^{n+1} - x_1^{n+1} = x_{N+1}^n - x_1^n,$$

(2.11) $$y_{N+1}^{n+1} - y_1^{n+1} = y_{N+1}^n - y_1^n.$$

We now define the discrete energy:

(2.12) $$E_\tau^n = \frac{1}{2} h \sum_{j=1}^{N} (\triangle_\tau^+ \theta_j^n)^2 + \frac{1}{2} h \sum_{j=1}^{N} (D_h^- \theta_j^n)(D_h^- \theta_j^{n+1})$$

$$+ \frac{1}{2} h \sum_{j=1}^{N} (\triangle_\tau^+ x_j^n)^2 + \frac{1}{2} h \sum_{j=1}^{N} (\triangle_\tau^+ y_j^n)^2.$$

LEMMA 1. (i) *For $n \geq 0$, we have $E_\tau^{n+1} = E_\tau^n$, and hence, $E_\tau^n = E_\tau^0$.*
(ii) *For every $n \geq 0$, E_τ^n is nonnegative and can be expressed in the form*

$$E_\tau^n = \frac{1}{4} h \sum_{j=1}^{N} (\triangle_\tau^+ \theta_j^n)^2 + \frac{1}{4} \frac{1}{h} \sum_{j=1}^{N} \left[(\theta_j^{n+1} - \theta_{j-1}^n)^2 + (\theta_j^n - \theta_{j-1}^{n+1})^2 \right]$$

$$+ \frac{1}{2} h \sum_{j=1}^{N} (\triangle_\tau^+ x_j^n)^2 + \frac{1}{2} h \sum_{j=1}^{N} (\triangle_\tau^+ y_j^n)^2.$$

(iii) *For $n \geq 0$,*

(2.13) $$\|D_h^- \theta_h^{n+1}\|_0^2 + |\theta_h^n|_e^2 \leq 24 E_\tau^n.$$

Proof. To show part (i), we multiply equation (1.11) by $h(\theta_j^{n+1} - \theta_j^{n-1})$ and sum j from 1 to N. Applying summation by parts to the second term on the left-hand side, using boundary condition (1.12), and simplifying, we have

$$\text{LHS} = h \sum_{j=1}^{N} (\triangle_\tau^+ \theta_j^n)^2 + h \sum_{j=1}^{N} (D_h^- \theta_j^n)(D_h^- \theta_j^{n+1})$$

$$- h \sum_{j=1}^{N} (\triangle_\tau^+ \theta_j^{n-1})^2 - h \sum_{j=1}^{N} (D_h^- \theta_j^{n-1})(D_h^- \theta_j^n).$$

For the first term on the right-hand side, we use equation (2.6) to substitute $\cos \theta_j^{n+1}$ and $\cos \theta_j^{n-1}$ and sum by parts. Using boundary condition (2.10), we have

$$h \sum_{j=1}^{N} f_j^n (\cos \theta_j^{n+1} - \cos \theta_j^{n-1}) = -\frac{1}{h} \sum_{j=1}^{N} (f_j^n - f_{j-1}^n)(x_j^{n+1} - x_j^{n-1}).$$

Applying equation (2.8), we find

$$h \sum_{j=1}^{N} f_j^n (\cos \theta_j^{n+1} - \cos \theta_j^{n-1}) = -h \sum_{j=1}^{N} (\triangle_\tau^+ x_j^n)^2 + h \sum_{j=1}^{N} (\triangle_\tau^+ x_j^{n-1})^2.$$

Using a similar treatment for the second term, we get

$$\text{RHS} = -h \sum_{j=1}^{N} (\triangle_\tau^+ x_j^n)^2 - h \sum_{j=1}^{N} (\triangle_\tau^+ y_j^n)^2 + h \sum_{j=1}^{N} (\triangle_\tau^+ x_j^{n-1})^2 + h \sum_{j=1}^{N} (\triangle_\tau^+ y_j^{n-1})^2.$$

Thus, we have conservation of the discrete energy

$$E_\tau^{n+1} = E_\tau^n \quad \text{for } n \geq 0.$$

To show part (ii), we first use boundary condition (1.12) and CFL condition (1.8) to write

$$\frac{1}{2} h \sum_{j=1}^{N} (\triangle_\tau^+ \theta_j^n)^2 + \frac{1}{2} h \sum_{j=1}^{N} (D_h^- \theta_j^n)(D_h^- \theta_j^{n+1})$$

$$= \frac{1}{2} \frac{h}{\tau^2} \left[\sum_{j=1}^{N} (\theta_j^{n+1} - \theta_j^n)^2 + \frac{1}{2} \sum_{j=1}^{N} (\theta_j^{n+1} - \theta_{j-1}^{n+1})(\theta_j^n - \theta_{j-1}^n) \right].$$

We then calculate

$$\frac{1}{2} \frac{h}{\tau^2} \left[\sum_{j=1}^{N} (\theta_j^{n+1} - \theta_j^n)^2 + \frac{1}{2} \sum_{j=1}^{N} (\theta_j^{n+1} - \theta_{j-1}^{n+1})(\theta_j^n - \theta_{j-1}^n) \right] = \frac{1}{2} \frac{h}{\tau^2} \left[\sum_{j=1}^{N} (\theta_j^{n+1} - \theta_j^n)^2 \right.$$

$$+ \sum_{j=1}^{N} \left(\theta_j^{n+1} \theta_j^n - \frac{1}{2} \theta_{j-1}^{n+1} \theta_j^n - \frac{1}{2} \theta_j^{n+1} \theta_{j-1}^n \right) + \frac{1}{2} (\theta_0^{n+1} \theta_0^n - \theta_N^{n+1} \theta_N^n) \Big]$$

$$= \frac{1}{2} \frac{h}{\tau^2} \left[\frac{1}{2} \sum_{j=1}^{N} (\theta_j^{n+1} - \theta_j^n)^2 + \frac{1}{2} \sum_{j=1}^{N} \left[(\theta_j^{n+1})^2 + (\theta_j^n)^2 - \theta_{j-1}^{n+1} \theta_j^n - \theta_j^{n+1} \theta_{j-1}^n \right] \right.$$

$$+ \frac{1}{2} (\theta_0^{n+1} \theta_0^n - \theta_N^{n+1} \theta_N^n) \Big]$$

$$= \frac{1}{2} \frac{h}{\tau^2} \left\{ \frac{1}{2} \sum_{j=1}^{N} (\theta_j^{n+1} - \theta_j^n)^2 + \frac{1}{4} \sum_{j=1}^{N} (\theta_j^n)^2 + \frac{1}{4} \sum_{j=1}^{N} (\theta_{j-1}^{n+1})^2 - \frac{1}{2} \sum_{j=1}^{N} \theta_{j-1}^{n+1} \theta_j^n \right.$$

$$+ \frac{1}{4} \sum_{j=1}^{N} (\theta_j^{n+1})^2 + \frac{1}{4} \sum_{j=1}^{N} (\theta_{j-1}^n)^2 - \frac{1}{2} \sum_{j=1}^{N} \theta_j^{n+1} \theta_{j-1}^n$$

$$+ \left[\frac{1}{4} (\theta_N^{n+1})^2 + \frac{1}{4} (\theta_N^{n+1})^2 - \frac{1}{2} \theta_N^{n+1} \theta_N^n \right] - \left[\frac{1}{4} (\theta_0^{n+1})^2 + \frac{1}{4} (\theta_0^{n+1})^2 - \frac{1}{2} \theta_0^{n+1} \theta_0^n \right] \right\}$$

$$= \frac{1}{4} h \sum_{j=1}^{N} (\triangle_\tau^+ \theta_j^n)^2 + \frac{1}{4} \frac{1}{h} \sum_{j=1}^{N} \left[(\theta_j^{n+1} - \theta_{j-1}^n)^2 + (\theta_j^n - \theta_{j-1}^{n+1})^2 \right].$$

In the last step, we used the equation $\theta_0^{n+1} - \theta_0^n = \theta_N^{n+1} - \theta_N^n$, which is a direct consequence of the boundary conditions $\theta_0^{n+1} + 2\pi = \theta_N^{n+1}$ and $\theta_0^n + 2\pi = \theta_N^n$.

Part (iii) can be easily derived by making use of the identities

$$\theta_j^n - \theta_{j-1}^n = (\theta_j^n - \theta_j^{n+1}) + (\theta_j^{n+1} - \theta_{j-1}^n),$$
$$\theta_j^{n+1} - \theta_{j-1}^{n+1} = (\theta_j^{n+1} - \theta_j^n) + (\theta_j^n - \theta_{j-1}^{n+1}).$$

In the proof of conservation of the discrete energy (on which much of the analysis of the approximation scheme depends), we have used the fact that approximate initial data can be found which satisfies the discrete compatibility conditions (1.16) and (1.17). We now show how such initial data can be determined which is also sufficiently close to the true solution.

LEMMA 2. *Let $\theta_0 \in C^4([0,1])$ and $\theta_1 \in C^3([0,1])$ satisfy conditions* (2.1), (2.2), *and* (2.3). *Let $\tilde{\theta} \in C^4([0,1] \times [0,T])$ for some $T > 0$ be the true solution of initial boundary value problem (IBVP)* (1.1)–(1.7). *We define*

$$\varphi_j = \theta_0(jh) \qquad \text{for } 1 \le j \le N.$$

Then, for τ sufficiently small, there exists a mesh function ψ_h such that for $1 \le j \le N$,

$$\psi_j - \tilde{\theta}(jh, \tau) = O(\tau^3),$$

and ψ_h satisfies equations (1.16) *and* (1.17).

Proof. We introduce the mesh function $\tilde{\varphi}_j$, $1 \le j \le N$, defined by

$$\tilde{\varphi}_j = \theta_0(jh) + \theta_1(jh)\tau + \frac{1}{2}\tilde{\theta}_{\tau\tau}(jh, 0)\tau^2 + \frac{1}{6}\tilde{\theta}_{\tau\tau\tau}(jh, 0)\tau^3.$$

Notice that $\tilde{\theta}_{\tau\tau}$ and $\tilde{\theta}_{\tau\tau\tau}$ can be expressed in terms of θ_0 and θ_1 and their derivatives. Let $\tilde{\theta}_j^n = \tilde{\theta}(jh, n\tau)$. Then, it is clear that for $1 \le j \le N$,

(2.14) $\tilde{\varphi}_j - \tilde{\theta}_j^1 = O(\tau^4).$

For any $\tau \ge 0$, since $\tilde{\theta}(0,\tau) + 2\pi = \tilde{\theta}(1,\tau)$, there exist $\xi_1, \xi_2 \in [0,1]$ (which may depend on τ) such that

$$\cos\tilde{\theta}(\xi_1, \tau) = 0, \qquad \sin\tilde{\theta}(\xi_2, \tau) = 0.$$

Hence, there is a $\tilde{\delta} > 0$, such that for $\tau \le \tilde{\delta}$, there exist $1 \le k, l \le N$, $k \ne l$ (which may depend on τ) such that

(2.15) $|\cos\tilde{\varphi}_k| \le \dfrac{1}{4}, \qquad |\sin\tilde{\varphi}_l| \le \dfrac{1}{4}.$

Now we define ψ_j as follows:

$$\psi_j = \tilde{\varphi}_j \qquad \text{if } j \ne k, l$$

and ψ_k and ψ_l are determined by the system (1.16) and (1.17). We claim that for τ sufficiently small, ψ_k and ψ_l are well defined and have the properties

$$\psi_k - \tilde{\theta}_k^1 = O(\tau^3), \qquad \psi_l - \tilde{\theta}_l^1 = O(\tau^3).$$

We begin by rewriting the system (1.16) and (1.17) as

(2.16) $(\cos\psi_k - \cos\tilde{\varphi}_k) + (\cos\psi_l - \cos\tilde{\varphi}_l) = \epsilon_1(\tau),$
(2.17) $(\sin\psi_k - \sin\tilde{\varphi}_k) + (\sin\psi_l - \sin\tilde{\varphi}_l) = \epsilon_2(\tau),$

where

$$\epsilon_1(\tau) = \sum_{j=1}^{N}(\cos \tilde\theta_j^0 - \cos \tilde\theta_j^1) - \sum_{j=1}^{N}(\cos \tilde\varphi_j - \cos \tilde\theta_j^1),$$

$$\epsilon_2(\tau) = \sum_{j=1}^{N}(\sin \tilde\theta_j^0 - \sin \tilde\theta_j^1) - \sum_{j=1}^{N}(\sin \tilde\varphi_j - \sin \tilde\theta_j^1).$$

To solve this system for ψ_k and ψ_l, we define

$$\psi^+ = (\psi_k + \psi_l)/2, \qquad \psi^- = (\psi_k - \psi_l)/2;$$
$$\tilde\phi^+ = (\tilde\phi_k + \tilde\phi_l)/2, \qquad \tilde\phi^- = (\tilde\phi_k - \tilde\phi_l)/2.$$

Then from simple trigonometric identities, we get:

$$2 \cos \psi^+ \cos \psi^- = 2 \cos \tilde\phi^+ \cos \tilde\phi^- + \epsilon_1,$$
$$2 \sin \psi^+ \cos \psi^- = 2 \sin \tilde\phi^+ \cos \tilde\phi^- + \epsilon_2.$$

Dividing these equations, we easily obtain

$$\tan \psi^+ = \frac{2 \sin \tilde\phi^+ \cos \tilde\phi^- + \epsilon_2}{\cos \tilde\phi^+ \cos \tilde\phi^- + \epsilon_1}.$$

We then choose

$$\psi^+ = \tan^{-1}\left[\frac{(2 \sin \tilde\phi^+ \cos \tilde\phi^- + \epsilon_2)}{(\cos \tilde\phi^+ \cos \tilde\phi^- + \epsilon_1)}\right] + m\pi,$$

where m is an integer determined by the condition $\tilde\phi^+ = \tan^{-1}(\tan \tilde\phi^+) + m\pi$. (Recall that the range of $\tan^{-1}$ is $[-\pi/2, \pi/2]$.)

Squaring and summing the original equations, applying a simple trigonometric identity, and simplifying the result, we also obtain

$$\cos(\psi_k - \psi_l) = \cos(\tilde\phi_k - \tilde\phi_l) + E_1,$$

where

$$E_1 \equiv \epsilon_1[\cos \tilde\phi_k + \cos \tilde\phi_l] + \epsilon_2[\sin \tilde\phi_k + \sin \tilde\phi_l] + \epsilon_1^2/2 + \epsilon_2^2/2.$$

Using (2.15), we get that

$$|\cos(\tilde\phi_k - \tilde\phi_l)| = |\cos \tilde\phi_k \cos \tilde\phi_l + \sin \tilde\phi_k \sin \tilde\phi_l| \leq \frac{1}{2},$$

and hence that

$$|\cos(\tilde\phi_k - \tilde\phi_l) + E_1| \leq \frac{1}{2} + \frac{5|\epsilon_1|}{4} + \frac{5|\epsilon_2|}{4} + \frac{\epsilon_1^2}{2} + \frac{\epsilon_2^2}{2} \leq 1$$

for ϵ_1 and ϵ_2 sufficiently small. We then choose

$$\psi^- = (\psi_k - \psi_l)/2 = \frac{1}{2}\{\cos^{-1}[\cos(\tilde\phi_k - \tilde\phi_l) + E_1] + n\pi\},$$

where n is an integer determined by the condition $\tilde{\phi}_k - \tilde{\phi}_l = \cos^{-1}[\cos(\tilde{\phi}_k - \tilde{\phi}_l)] + n\pi$. (Recall that the range of $\cos^{-1}$ is $[0, \pi]$.) Hence, $\psi_k = \psi^+ + \psi^-$ and $\psi_l = \psi^+ - \psi^-$ are determined.

We next show that $\psi_j - \tilde{\theta}(jh, \tau) = O(\tau^3)$. Using our previous results, we get

$$\tan \psi^+ - \tan \tilde{\phi}^+ = \frac{2 \sin \tilde{\phi}^+ \cos \tilde{\phi}^- + \epsilon_2}{2 \cos \tilde{\phi}^+ \cos \tilde{\phi}^- + \epsilon_1} - \frac{\sin \tilde{\phi}^+ \cos \tilde{\phi}^-}{\cos \tilde{\phi}^+ \cos \tilde{\phi}^-}$$

$$= \frac{\epsilon_2 \cos \tilde{\phi}^+ \cos \tilde{\phi}^- - \epsilon_1 \sin \tilde{\phi}^+ \cos \tilde{\phi}^-}{(2 \cos \tilde{\phi}^+ \cos \tilde{\phi}^- + \epsilon_1)(\cos \tilde{\phi}^+ \cos \tilde{\phi}^-)} \equiv E_2.$$

Now $2 \cos \tilde{\phi}^+ \cos \tilde{\phi}^- = \cos \tilde{\phi}_k + \cos \tilde{\phi}_l$, and by (2.15),

$$|\cos \tilde{\phi}_k| \leq \frac{1}{4}, \qquad |\cos \tilde{\phi}_l| = \sqrt{1 - \sin^2 \tilde{\phi}_l} \geq \frac{\sqrt{15}}{4}.$$

Hence, for ϵ_1 and ϵ_2 sufficiently small, it easily follows that $|E_2| \leq C(|\epsilon_1| + |\epsilon_2|)$. Now by the mean value theorem, there exists a β such that

$$|\tan \psi^+ - \tan \tilde{\phi}^+| = |\sec^2 \beta||\psi^+ - \tilde{\phi}^+|.$$

(Note that ψ^+ and $\tilde{\phi}^+$ belong to the same branch of the tangent.) Hence,

$$|\psi^+ - \tilde{\phi}^+| \leq |\cos^2 \beta||\tan \psi^+ - \tan \tilde{\phi}^+| \leq |E_2| \leq C(|\epsilon_1| + |\epsilon_2|).$$

Finally, from the identity $\cos(\psi_k - \psi_l) = \cos(\tilde{\phi}_k - \tilde{\phi}_l) + E_1$ and the mean value theorem, we get

$$\cos^{-1}[\cos(\psi_k - \psi_l)] = \cos^{-1}[\cos(\tilde{\phi}_k - \tilde{\phi}_l) + E_1] = \cos^{-1}[\cos(\tilde{\phi}_k - \tilde{\phi}_l)] - E_1(1 - \xi^2)^{-\frac{1}{2}},$$

where ξ satisfies $|\cos(\tilde{\phi}_k - \tilde{\phi}_l) - \xi| \leq |E_1|$. Since $|\cos(\tilde{\phi}_k - \tilde{\phi}_l)| \leq 1/2$ and $|E_1| \leq C(|\epsilon_1| + |\epsilon_2|)$, we get for $|\epsilon_1|$ and $|\epsilon_2|$ sufficiently small that $|\xi| \leq 3/4$. Hence,

$$|\psi^- - \tilde{\phi}^-| = 2|(\psi_k - \psi_l) - (\tilde{\phi}_k - \tilde{\phi}_l)|$$
$$= 2|\cos^{-1}[\cos(\psi_k - \psi_l)] - \cos^{-1}[\cos(\tilde{\phi}_k - \tilde{\phi}_l)]| \leq C|E_1| \leq C(|\epsilon_1| + |\epsilon_2|).$$

Since

$$|\psi_k - \tilde{\phi}_k| \leq |\psi^+ - \tilde{\phi}^+| + |\psi^- - \tilde{\phi}^-|, \qquad |\psi_l - \tilde{\phi}_l| \leq |\psi^+ - \tilde{\phi}^+| + |\psi^- - \tilde{\phi}^-|$$

to obtain the desired error estimate, we need only show that ϵ_1 and ϵ_2 are $O(\tau^3)$.

Since $\tilde{\theta} \in C^4([0, 1] \times [0, T])$, it follows from equation (1.3) and boundary conditions (1.4), (1.5), and (1.6) that

(2.18) $\tilde{\theta}_{ss}(0, t) = \tilde{\theta}_{ss}(1, t), \qquad \tilde{\theta}_{sss}(0, t) = \tilde{\theta}_{sss}(1, t).$

Integrating equations (1.1) and (1.2) with respect to s over $[0,1]$ and applying boundary conditions (1.5) and (1.6), we find that for any $\tau > 0$,

(2.19) $$\int_0^1 \cos \tilde{\theta}(s, \tau) ds = \int_0^1 \cos \tilde{\theta}(s, 0) ds,$$

(2.20) $$\int_0^1 \sin \tilde{\theta}(s, \tau) ds = \int_0^1 \sin \tilde{\theta}(s, 0) ds.$$

Using (2.18), (2.19), and (2.20), we employ the Euler–Maclaurin summation formula [4, pp. 297–302] to obtain

$$\sum_{j=1}^{N} \cos \tilde{\theta}_j^0 - \sum_{j=1}^{N} \cos \tilde{\theta}_j^1 = O(\tau^3),$$

$$\sum_{j=1}^{N} \sin \tilde{\theta}_j^0 - \sum_{j=1}^{N} \sin \tilde{\theta}_j^1 = O(\tau^3).$$

Hence, ϵ_1 and ϵ_2 are of order τ^3; i.e., there is a constant $A \geq 0$, which depends on the initial data and the third- and fourth-order derivatives of the exact solution in a neighborhood of $t = 0$, such that for τ sufficiently small,

$$|\epsilon_1(\tau)| \leq A\tau^3, \qquad |\epsilon_2(\tau)| \leq A\tau^3.$$

Combining our results completes the proof of the lemma.

3. Semilinear form. The most important step in deriving a convergent iteration scheme for obtaining the approximate solution (and also proving its existence) is to eliminate $\{f_j^n\}$ and $\{g_j^n\}$ and to rewrite the system (1.9)–(1.14) as a single semilinear equation for $\{\theta_j^n\}$. We begin with solving equations (1.9) and (1.10) to express f_j^n and g_j^n in terms of $\{\theta_j^n\}$. Let $\{K_{ij}\}$ be the discrete Green function defined by the following: for $0 \leq j \leq N$,

(3.1)
$$K_{ij} = \begin{cases} hi(1 - hj) & \text{if } 0 \leq i \leq j - 1, \\ hj(1 - hi) & \text{if } j \leq i \leq N. \end{cases}$$

Then, we can write for $1 \leq j \leq N$,

(3.2)
$$f_j^n = \hat{f}^n - h \sum_{i=1}^{N} K_{ij} \Delta_\tau^2 \cos \theta_i^n,$$

(3.3)
$$g_j^n = \hat{g}^n - h \sum_{i=1}^{N} K_{ij} \Delta_\tau^2 \sin \theta_i^n,$$

where

$$\hat{f}^n \equiv f_0^n = f_N^n, \qquad \hat{g}^n \equiv g_0^n = g_N^n,$$

with the compatibility conditions: for $n \geq 1$,

(3.4)
$$\sum_{j=1}^{N} \Delta_\tau^2 \cos \theta_j^n = 0, \qquad \sum_{j=1}^{N} \Delta_\tau^2 \sin \theta_j^n = 0.$$

Next, we introduce some notation and prove a lemma which we need in the next step. Define

$$S^n(\theta_j) = \int_0^1 \sin(\eta \theta_j^{n+1} + (1 - \eta)\theta_j^{n-1}) d\eta$$
$$= \begin{cases} -\left(\cos \theta_j^{n+1} - \cos \theta_j^{n-1}\right) / \left(\theta_j^{n+1} - \theta_j^{n-1}\right) & \text{if } \theta_j^{n+1} \neq \theta_j^{n-1}, \\ \sin \theta_j^{n-1} & \text{if } \theta_j^{n+1} = \theta_j^{n-1}; \end{cases}$$

$$C^n(\theta_j) = \int_0^1 \cos(\eta\theta_j^{n+1} + (1-\eta)\theta_j^{n-1})d\eta$$

$$= \begin{cases} (\sin\theta_j^{n+1} - \sin\theta_j^{n-1})/(\theta_j^{n+1} - \theta_j^{n-1}) & \text{if } \theta_j^{n+1} \neq \theta_j^{n-1}, \\ \cos\theta_j^{n-1} & \text{if } \theta_j^{n+1} = \theta_j^{n-1}; \end{cases}$$

$$\tilde{S}^n(\theta_j) = 2\int_0^1\int_0^1 \xi\sin\left(\eta\xi\theta_j^{n+1} + (1-\eta)\xi\theta_j^n + (1-\xi)\theta_j^{n-1}\right)d\eta d\xi;$$

$$\tilde{C}^n(\theta_j) = 2\int_0^1\int_0^1 \xi\cos\left(\eta\xi\theta_j^{n+1} + (1-\eta)\xi\theta_j^n + (1-\xi)\theta_j^{n-1}\right)d\eta d\xi;$$

$$\check{S}^n(\theta_i,\theta_j) = -S^n(\theta_j)\tilde{C}^n(\theta_i) + C^n(\theta_j)\tilde{S}^n(\theta_i);$$

$$\hat{C}^n(\theta_i,\theta_j) = S^n(\theta_j)S^n(\theta_i) + C^n(\theta_j)C^n(\theta_i).$$

LEMMA 3. *For $1 \leq j \leq N$ and $n \geq 1$, we have*

$$\triangle_\tau^2\cos\theta_j^n = -S^n(\theta_j)\triangle_\tau^2\theta_j^n - \tilde{C}^n(\theta_j)\triangle_\tau^+\theta_j^n\triangle_\tau^+\theta_j^{n-1},$$

$$\triangle_\tau^2\sin\theta_j^n = C^n(\theta_j)\triangle_\tau^2\theta_j^n - \tilde{S}^n(\theta_j)\triangle_\tau^+\theta_j^n\triangle_\tau^+\theta_j^{n-1}.$$

Proof. We calculate

$$\triangle_\tau^2\cos\theta_j^n + S^n(\theta_j)\triangle_\tau^2\theta_j^n$$

$$= -\frac{1}{\tau^2}\frac{1}{\theta_j^{n+1} - \theta_j^{n-1}}\Big[(\cos\theta_j^{n+1} - \cos\theta_j^{n-1})(\theta_j^{n+1} - 2\theta_j^n + \theta_j^{n-1})$$

$$-(\cos\theta_j^{n+1} - 2\cos\theta_j^n + \cos\theta_j^{n-1})(\theta_j^{n+1} - \theta_j^{n-1})\Big]$$

$$= -\frac{1}{\tau^2}\frac{2}{\theta_j^{n+1} - \theta_j^{n-1}}\Big[-(\cos\theta_j^{n+1} - \cos\theta_j^{n-1})(\theta_j^n - \theta_j^{n-1})$$

$$+(\cos\theta_j^n - \cos\theta_j^{n-1})(\theta_j^{n+1} - \theta_j^{n-1})\Big]$$

$$= -\frac{2}{\tau^2}(\theta_j^n - \theta_j^{n-1})\int_0^1\Big[\sin(\xi\theta_j^{n+1} + (1-\xi)\theta_j^{n-1}) - \sin(\xi\theta_j^n + (1-\xi)\theta_j^{n-1})\Big]d\xi$$

$$= -\frac{2}{\tau^2}(\theta_j^n - \theta_j^{n-1})(\theta_j^{n+1} - \theta_j^n)$$

$$\times \int_0^1\int_0^1 \xi\cos\left(\eta\xi\theta_j^{n+1} + (1-\eta)\xi\theta_j^n + (1-\xi)\theta_j^{n-1}\right)d\eta d\xi$$

$$= -\tilde{C}^n(\theta_j)\triangle_\tau^+\theta_j^{n-1}\triangle_\tau^+\theta_j^n.$$

The other formula can be proven in the same way.

Now, we put (3.2), (3.3) into equation (1.11) and apply Lemma 3 to obtain for $1 \leq j \leq N$,

$$\triangle_\tau^2\theta_j^n - \triangle_h^2\theta_j^n = -\hat{f}^n S^n(\theta_j) + \hat{g}^n C^n(\theta_j) - h\sum_{i=1}^N K_{ij}\hat{C}^n(\theta_i,\theta_j)\triangle_\tau^2\theta_i^n$$

(3.5)
$$+ h\sum_{i=1}^N K_{ij}\check{S}^n(\theta_i,\theta_j)\triangle_\tau^+\theta_i^n\triangle_\tau^+\theta_i^{n-1}.$$

To find the semilinear equation for $\{\theta_j^n\}$, we observe that a $\triangle_h^2\theta_i^n$ term is needed to accompany the $\triangle_\tau^2\theta_i^n$ inside of the first summation on the right-hand side of (3.5). Toward this end, we use summation by parts and boundary condition $K_{Nj} = K_{0j} = 0$ to derive for $1 \leq j \leq N$,

$$h\sum_{i=1}^{N}K_{ij}\hat{C}^n(\theta_i,\theta_j)\triangle_h^2\theta_i^n = -\frac{1}{h}\sum_{i=1}^{N}(K_{ij} - K_{i-1,j})\hat{C}^n(\theta_i,\theta_j)(\theta_i^n - \theta_{i-1}^n)$$

(3.6)
$$-\frac{1}{h}\sum_{i=2}^{N}K_{i-1,j}(\hat{C}^n(\theta_i,\theta_j) - \hat{C}^n(\theta_{i-1},\theta_j))(\theta_i^n - \theta_{i-1}^n).$$

Now combining (3.6) and (3.5), we obtain

$$\triangle_\tau^2\theta_j^n - \triangle_h^2\theta_j^n + h\sum_{i=1}^{N}K_{ij}\hat{C}^n(\theta_i,\theta_j)(\triangle_\tau^2\theta_i^n - \triangle_h^2\theta_i^n)$$

$$= -\hat{f}^nS^n(\theta_j) + \hat{g}^nC^n(\theta_j) + h\sum_{i=1}^{N}K_{ij}\check{S}^n(\theta_i,\theta_j)\triangle_\tau^+\theta_i^n\triangle_\tau^+\theta_i^{n-1}$$

$$+\frac{1}{h}\sum_{i=2}^{N}K_{i-1,j}(\hat{C}^n(\theta_i,\theta_j) - \hat{C}^n(\theta_{i-1},\theta_j))(\theta_i^n - \theta_{i-1}^n)$$

$$+\frac{1}{h}\sum_{i=1}^{N}(K_{ij} - K_{i-1,j})\hat{C}^n(\theta_i,\theta_j)(\theta_i^n - \theta_{i-1}^n).$$

We then use the boundary conditions $\theta_0^n = \theta_N^n - 2\pi$ and $\theta_{N+1}^n = \theta_1^n + 2\pi$ to eliminate θ_0^n and θ_{N+1}^n. The above equation can be written in terms of $\theta_1^n,\ldots,\theta_N^n$ and the operators D_h^2 and D_h^- defined at the end of §1:

$$\left(\triangle_\tau^2\theta_h^n - D_h^2\theta_h^n\right) + \mathbf{L}_{\theta_h}^n\left(\triangle_\tau^2\theta_h^n - D_h^2\theta_h^n\right) = \mathbf{A}^n(\theta_h),$$

in which

(3.7)
$$(\mathbf{L}_{\theta_h}^n u_h)_j = h\sum_{i=1}^{N}K_{ij}\hat{C}^n(\theta_i,\theta_j)u_i,$$

$$\mathbf{B}^n(\theta_h)_j = h\sum_{i=1}^{N}K_{ij}\check{S}^n(\theta_i,\theta_j)\triangle_\tau^+\theta_i^n\triangle_\tau^+\theta_i^{n-1}$$

(3.8)
$$+h\sum_{i=2}^{N}K_{i-1,j}\frac{1}{h}(\hat{C}^n(\theta_i,\theta_j) - \hat{C}^n(\theta_{i-1},\theta_j))D_h^-\theta_i^n$$

$$+h\sum_{i=1}^{N}\frac{1}{h}(K_{ij} - K_{i-1,j})\hat{C}^n(\theta_i,\theta_j)D_h^-\theta_i^n,$$

(3.9)
$$\mathbf{A}^n(\theta_h) = -\hat{f}^nS^n(\theta_h) + \hat{g}^nC^n(\theta_h) + \mathbf{B}^n(\theta_h).$$

Note that $\mathbf{A}^n(\theta_h)$ contains no second-order differences. The quantities $\hat{f}^n$ and $\hat{g}^n$ can be expressed in terms of θ_h and its first-order differences; the calculation is described at the end of this section.

The operator $\mathbf{L}_{\theta_h}^n$ is analyzed in the next section, and in particular it is shown that

$$(3.10) \qquad (\mathbf{I} + \mathbf{L}_{\theta_h}^n)^{-1} = \mathbf{I} + \mathbf{K}_{\theta_h}^n.$$

Accordingly, θ_h satisfies the equation

$$(3.11) \qquad \triangle_\tau^2 \theta_h^n - D_h^2 \theta_h^n = (\mathbf{I} + \mathbf{K}_{\theta_h}^n)\mathbf{A}^n(\theta_h).$$

Equation (3.11) is the main result of this section. It is a semilinear equation since the right-hand side does not involve second-order differences, and it is equivalent to (1.9)–(1.14).

At this point, we determine $\hat{f}^n$ and $\hat{g}^n$ in terms of θ_h. First let us suppose that θ_h, $\hat{f}^n$, and $\hat{g}^n$ form a solution triple to equation (3.11). Identity (3.9) implies that

$$\triangle_\tau^2 \theta_h^n - D_h^2 \theta_h^n = -\hat{f}^n(\mathbf{I} + \mathbf{K}_{\theta_h}^n)S^n(\theta_h) + \hat{g}^n(\mathbf{I} + \mathbf{K}_{\theta_h}^n)C^n(\theta_h) + (\mathbf{I} + \mathbf{K}_{\theta_h}^n)\mathbf{B}^n(\theta_h).$$

Multiplying this equation by $hS^n(\theta_h)^T$ and $hC^n(\theta_h)^T$, respectively, and summing by parts, we obtain the relations

$$
\begin{aligned}
&-hS^n(\theta_h)^T \triangle_\tau^2 \theta_h^n - h\sum_{j=1}^N \tilde{D}_h^- S^n(\theta_j)D_h^- \theta_j^n \\
(3.12) \qquad &= a_{11}^n(\theta_h)\hat{f}^n + a_{12}^n(\theta_h)\hat{g}^n - hS^n(\theta_h)^T(\mathbf{I} + \mathbf{K}_{\theta_h}^n)\mathbf{B}^n(\theta_h),
\end{aligned}
$$

$$
\begin{aligned}
&-hC^n(\theta_h)^T \triangle_\tau^2 \theta_h^n - h\sum_{j=1}^N \tilde{D}_h^- C^n(\theta_j)D_h^- \theta_j^n \\
(3.13) \qquad &= a_{21}^n(\theta_h)\hat{f}^n + a_{22}^n(\theta_h)\hat{g}^n - hC^n(\theta_h)^T(\mathbf{I} + \mathbf{K}_{\theta_h}^n)\mathbf{B}^n(\theta_h),
\end{aligned}
$$

where

$$(3.14) \qquad a_{11}^n(\theta_h) = hS^n(\theta_h)^T(\mathbf{I} + \mathbf{K}_{\theta_h}^n)S^n(\theta_h),$$
$$(3.15) \qquad a_{12}^n(\theta_h) = -hS^n(\theta_h)^T(\mathbf{I} + \mathbf{K}_{\theta_h}^n)C^n(\theta_h),$$
$$(3.16) \qquad a_{21}^n(\theta_h) = hC^n(\theta_h)^T(\mathbf{I} + \mathbf{K}_{\theta_h}^n)S^n(\theta_h),$$
$$(3.17) \qquad a_{22}^n(\theta_h) = -hC^n(\theta_h)^T(\mathbf{I} + \mathbf{K}_{\theta_h}^n)C^n(\theta_h).$$

In the next section, it is shown that for $h > 0$, $\mathbf{I} + \mathbf{K}_{\theta_h}^n$ is a positive definite operator on $\mathbb{R}^N$ and that for $h > 0$ sufficiently small and for any $n \geq 1$,

$$a_{11}^n(\theta_h)a_{22}^n(\theta_h) - a_{12}^n(\theta_h)a_{21}^n(\theta_h) < 0.$$

Hence, the system (3.12) and (3.13) uniquely determines $\hat{f}^n$ and $\hat{g}^n$.

Now the required solution θ_h must satisfy the compatibility condition (3.4), and must therefore satisfy the following equivalent forms, which are the results of Lemma 3; namely,

$$(3.18) \qquad S^n(\theta_h)^T \triangle_\tau^2 \theta_h^n = -\sum_{j=1}^N \tilde{C}^n(\theta_j)\triangle_\tau^+ \theta_j^n \triangle_\tau^+ \theta_j^{n-1},$$

$$(3.19) \qquad C^n(\theta_h)^T \triangle_\tau^2 \theta_h^n = \sum_{j=1}^N \tilde{S}^n(\theta_j)\triangle_\tau^+ \theta_j^n \triangle_\tau^+ \theta_j^{n-1}.$$

Accordingly, if we assume a priori that $\hat{f}^n$ and $\hat{g}^n$ have the dependence on θ_h given by the system

$$a_{11}^n(\theta_h)\hat{f}^n + a_{12}^n(\theta_h)\hat{g}^n = h\sum_{j=1}^N \tilde{C}^n(\theta_j)\triangle_\tau^+\theta_j^n\triangle_\tau^+\theta_j^{n-1}$$

(3.20)
$$-h\sum_{j=1}^N \tilde{D}_h^- S^n(\theta_j)D_h^-\theta_j^n + hS^n(\theta_h)^T(\mathbf{I}+\mathbf{K}_{\theta_h}^n)\mathbf{B}^n(\theta_h),$$

$$a_{21}^n(\theta_h)\hat{f}^n + a_{22}^n(\theta_h)\hat{g}^n = -h\sum_{j=1}^N \hat{S}^n(\theta_j)\triangle_\tau^+\theta_j^n\triangle_\tau^+\theta_j^{n-1}$$

(3.21)
$$-h\sum_{j=1}^N \tilde{D}_h^- C^n(\theta_j)D_h^-\theta_j^n + hC^n(\theta_h)^T(\mathbf{I}+\mathbf{K}_{\theta_h}^n)\mathbf{B}^n(\theta_h),$$

and solve equation (3.11) as a function of θ_h only, we are guaranteed that the solution arising satisfies compatibility condition (3.4). This statement is a consequence of the fact that (3.12), (3.20) together and (3.13), (3.21) together imply (3.18) and (3.19).

4. Analysis of the semilinear equation. We next present an analysis of $\mathbf{L}_{\theta_h}^n$ and $\mathbf{K}_{\theta_h}^n$, and some bounds on $\mathbf{A}^n(\theta_h)$. We also derive a lower bound for the absolute value of the determinant of the system (3.20) and (3.21). This bound is used to show that $\hat{f}^n$ and $\hat{g}^n$ are uniquely determined and to obtain a priori estimates for these quantities.

Recall that for any mesh function θ_h, the operators $\mathbf{L}_{\theta_h}^n$ and $\mathbf{K}_{\theta_h}^n$ are defined by (3.7) and (3.10), where K_{ij} is defined in (3.1). The operator $\mathbf{L}_{\theta_h}^n$ maps $\mathbb{R}^N$ to $\mathbb{R}^N$ and satisfies

(4.1)
$$\|\mathbf{L}_{\theta_h}^n u_h\|_\infty \leq \|u_h\|_0.$$

Since K_{ij} and $\tilde{C}^n(\theta_i,\theta_j)$ are symmetric in i and j, $\mathbf{L}_{\theta_h}^n$ is symmetric. For any mesh functions θ_h and φ_h, it is not difficult to show

(4.2) $$\|(\mathbf{L}_{\theta_h}^n - \mathbf{L}_{\varphi_h}^n)u_h\|_\infty \leq 2(\|\theta_h^{n+1}-\varphi_h^{n+1}\|_\infty + \|\theta_h^{n-1}-\varphi_h^{n-1}\|_\infty)\|u_h\|_0.$$

To show that $\mathbf{L}_{\theta_h}^n$ is positive semidefinite, we calculate

$$h\sum_{j=1}^N v_j(\mathbf{L}_{\theta_h}^n v_h)_j = h^2\sum_{j=1}^{N-1}\sum_{i=1}^{N-1} K_{ij}(C^n(\theta_i)C^n(\theta_j) + S^n(\theta_i)S^n(\theta_j))v_i v_j$$

$$= h^2\sum_{j=1}^{N-1}\sum_{i=1}^{N-1} K_{ij}\alpha_i\alpha_j + h^2\sum_{j=1}^{N-1}\sum_{i=1}^{N-1} K_{ij}\beta_i\beta_j \geq 0,$$

where

$$\alpha_j = C^n(\theta_j)v_j, \quad \beta_j = S^n(\theta_j)v_j.$$

Here we have used the equation $K_{iN} = K_{Nj} = 0$ for $1 \leq i,j \leq N$. The last step follows from the fact that $K_{ij},\ 0 \leq i,j \leq N$ is the discrete Green function for the BVP:

$$-\triangle_h^2 u_j = w_j, \quad u_0 = u_N = 0.$$

Hence, summation by parts yields that $\sum_{j=1}^{N-1}\sum_{i=1}^{N-1} K_{ij}w_iw_j \geq 0$ for any mesh function $\{w_j\}$.

It follows from the inequality $1 \leq \mathbf{I} + \mathbf{L}_{\theta_h}^n \leq 2$ that $(\mathbf{I} + \mathbf{K}_{\theta_h}^n) = (\mathbf{I} + \mathbf{L}_{\theta_h}^n)^{-1}$ is well defined. Moreover, $\mathbf{K}_{\theta_h}^n$ is symmetric, negative, semidefinite and satisfies

$$(4.3) \qquad\qquad \frac{1}{2} \leq \mathbf{I} + \mathbf{K}_{\theta_h}^n \leq 1.$$

It follows from the equation $\mathbf{K}_{\theta_h}^n = -\mathbf{L}_{\theta_h}^n(\mathbf{I} + \mathbf{L}_{\theta_h}^n)^{-1}$ that

$$(4.4) \qquad\qquad \|\mathbf{K}_{\theta_h}^n u_h\|_\infty \leq \|u_h\|_0.$$

Furthermore, for any mesh function θ_h and φ_h, since

$$\mathbf{K}_{\theta_h}^n - \mathbf{K}_{\varphi_h}^n = (\mathbf{I} + \mathbf{L}_{\varphi_h}^n)^{-1}(\mathbf{L}_{\varphi_h}^n - \mathbf{L}_{\theta_h}^n)(\mathbf{I} + \mathbf{L}_{\theta_h}^n)^{-1},$$

$\mathbf{K}_{\theta_h}^n$ is continuous in θ_h and satisfies

$$(4.5) \quad \|(\mathbf{K}_{\theta_h}^n - \mathbf{K}_{\varphi_h}^n)u_h\|_\infty \leq 4(\|\theta_h^{n+1} - \varphi_h^{n+1}\|_\infty + \|\theta_h^{n-1} - \varphi_h^{n-1}\|_\infty)\|u_h\|_0.$$

In order to show that the approximation scheme is well defined, we need to show that $\hat{f}^n$ and $\hat{g}^n$ are uniquely determined by the system (3.20) and (3.21). We now show how this can be done. For future reference, we state the following hypothesis.

Hypothesis (H). For each $n \geq 0$, there exists a $\delta_n > 0$ such that for $0 < h < \delta_n$,

$$h(4\|\triangle_\tau^+\theta_h^n\|_0^2 + 4\|\triangle_\tau^+\theta_h^{n-1}\|_0^2 + 2\|D_h^-\theta_h^{n-1}\|_0^2) \leq \frac{1}{32}.$$

The key step is the following technical lemma, which is then used to give a lower bound for the determinant of the system defining $\hat{f}^n$ and $\hat{g}^n$.

LEMMA 4. *Suppose that $\hat{\theta}^n$ is a function of n which satisfies Hypothesis* (H). *Then, for $0 < h < \delta_n$, we have*

$$h\sum_{j=1}^{N}\left[\frac{\cos(\theta_j^{n+1} - \hat{\theta}^n) - \cos(\theta_j^{n-1} - \hat{\theta}^n)}{\theta_j^{n+1} - \theta_j^{n-1}}\right]^2$$

$$\geq \frac{1}{64(1 + 4\|\triangle_\tau^+\theta_h^n\|_0^2 + 4\|\triangle_\tau^+\theta_h^{n-1}\|_0^2 + 2\|D_h^-\theta_h^{n-1}\|_0^2)}.$$

Proof. Fix $n \geq 1$. We write for $1 \leq j \leq N$,

$$(4.6) \qquad -\frac{\cos(\theta_j^{n+1} - \hat{\theta}^n) - \cos(\theta_j^{n-1} - \hat{\theta}^n)}{\theta_j^{n+1} - \theta_j^{n-1}} = \sin(\varphi_j^n - \hat{\theta}^n),$$

where

$$\varphi_j^n = \xi_j^n\theta_j^{n+1} + (1 - \xi_j^n)\theta_j^{n-1} \quad \text{for some} \quad \xi_j^n \in [0, 1].$$

A direct calculation shows that

$$\|D_h^-\varphi_j^n\|_0^2 \leq \frac{1}{h}\sum_{j=2}^{N}(\varphi_j^n - \varphi_{j-1}^n)^2 + \frac{1}{h}(\varphi_1^n - \varphi_N^n + 2\pi)^2$$

$$= \frac{1}{h} \sum_{j=2}^{N} \left[\xi_j^n (\theta_j^{n+1} - \theta_j^{n-1}) - \xi_{j-1}^n (\theta_{j-1}^{n+1} - \theta_{j-1}^{n-1}) + (\theta_j^{n-1} - \theta_{j-1}^{n-1}) \right]^2$$

$$+ \frac{1}{h} \left[\xi_1^n (\theta_1^{n+1} - \theta_1^{n-1}) - \xi_N^n (\theta_N^{n+1} - \theta_N^{n-1}) + (\theta_1^{n-1} - \theta_N^{n-1} + 2\pi) \right]^2$$

$$\leq \frac{2}{h} \sum_{j=2}^{N} \left[(\theta_j^{n+1} - \theta_j^{n-1})^2 + (\theta_{j-1}^{n+1} - \theta_{j-1}^{n-1})^2 + (\theta_j^{n-1} - \theta_{j-1}^{n-1})^2 \right]$$

$$+ \frac{2}{h} \left[(\theta_1^{n+1} - \theta_1^{n-1})^2 + (\theta_N^{n+1} - \theta_N^{n-1})^2 + (\theta_1^{n-1} - \theta_N^{n-1} + 2\pi)^2 \right]$$

$$(4.7) \qquad \leq 4 \| \triangle_\tau^+ \theta_h^n \|_0^2 + 4 \| \triangle_\tau^+ \theta_h^{n-1} \|_0^2 + 2 \| D_h^- \theta_h^{n-1} \|_0^2 \equiv (M_h^n)^2.$$

It follows that

$$\max \left(\max_{2 \leq j \leq N} |\varphi_j^n - \varphi_{j-1}^n|, \quad |\varphi_1^n - \varphi_N^n + 2\pi| \right) \leq \sqrt{h} M_h^n.$$

Let $\varphi_n^* \in [\varphi_N^n - 2\pi, \varphi_N^n)$ be such that

$$\sin(\varphi_n^* - \hat{\theta}^n) = 1,$$

and denote by j_h, an integer between 1 and N, such that

$$|\varphi_n^* - \varphi_{j_h}^n| \leq \sqrt{h} M_h^n.$$

Then, using Hypothesis (H), there exists a $\delta_n > 0$ such that for $0 < h < \delta_n$,

$$\sqrt{h} M_h^n \leq \frac{1}{4}.$$

Hence, for $0 < h < \delta_n$, we have

$$\sin(\varphi_{j_h}^n - \hat{\theta}^n) \geq \frac{3}{4}.$$

Now, we calculate for $j_h + 1 \leq j \leq N$,

$$\sin(\varphi_j^n - \hat{\theta}^n) = \sin \left((\varphi_{j_h}^n - \hat{\theta}^n) + \sum_{i=j_h+1}^{j} (\varphi_i^n - \varphi_{i-1}^n) \right)$$

$$\geq \frac{3}{4} - \left| \sum_{i=j_h+1}^{j} (\varphi_i^n - \varphi_{i-1}^n) \right| \geq \frac{3}{4} - h^{\frac{1}{2}} |j - j_h|^{\frac{1}{2}} \| D_h^- \varphi_h^n \|_0.$$

The same inequality holds for $1 \leq j \leq j_h$. Hence, for $1 \leq j \leq N$,

$$(4.8) \qquad \sin(\varphi_j^n - \hat{\theta}^n) \geq \frac{3}{4} - h^{\frac{1}{2}} |j - j_h|^{\frac{1}{2}} \| D_h^- \varphi_h^n \|_0.$$

Let N_h denote the integer such that

$$\frac{1}{16(1 + \| D_h^- \varphi_h^n \|_0^2) h} - 1 \leq N_h \leq \frac{1}{16(1 + \| D_h^- \varphi_h^n \|_0^2) h}.$$

Note that $N_h \leq N/4$. Then, for all j such that $|j - j_h| \leq N_h$,

$$\left[h|j - j_h|(1 + \|D_h^- \varphi_h^n\|_0^2)\right]^{\frac{1}{2}} \leq \frac{1}{4}.$$

It follows from (4.8) that for $|j - j_h| \leq N_h$,

$$\sin(\varphi_j^n - \hat{\theta}^n) \geq \frac{1}{2}.$$

We now observe that either

$$h \sum_{j=1}^{N} \sin^2(\varphi_j^n - \hat{\theta}^n) \geq h \sum_{j=j_h}^{j_h+N_h} \sin^2(\varphi_j^n - \hat{\theta}^n) \geq \frac{h}{4}(N_h + 1)$$

or

$$h \sum_{j=1}^{N} \sin^2(\varphi_j^n - \hat{\theta}^n) \geq h \sum_{j=j_h-N_h}^{j_h} \sin^2(\varphi_j^n - \hat{\theta}^n) \geq \frac{h}{4}(N_h + 1).$$

But the definition of N_h implies

$$h(N_h + 1) \geq \frac{1}{16(1 + \|D_h^- \varphi_h^n\|_0^2)}.$$

Hence, we obtain

$$h \sum_{j=1}^{N} \sin^2(\varphi_j^n - \hat{\theta}^n) \geq \frac{1}{64(1 + \|D_h^- \varphi_h^n\|_0^2)}.$$

The conclusion of the lemma follows from (4.6) and (4.7).

We are now ready to derive a lower bound for the determinant of the system defining $\hat{f}^n$ and $\hat{g}^n$. From this result, it is easy to see that these quantities are well defined, and bounds for $\hat{f}^n$ and $\hat{g}^n$ may then be obtained in a straightforward manner.

LEMMA 5. *If Hypothesis* (H) *holds, then*

$$|a_{11}^n(\theta_h)a_{22}^n(\theta_h) - a_{12}^n(\theta_h)a_{21}^n(\theta_h)|$$
$$\geq \frac{1}{2^{14}} \frac{1}{(1 + 4\|\triangle_\tau^+ \theta_h^n\|_0^2 + 4\|\triangle_\tau^+ \theta_h^{n-1}\|_0^2 + 2\|D_h^- \theta_h^{n-1}\|_0^2)^2},$$

where $a_{ij}^n(\theta_h)$, $1 \leq i, j \leq 2$, are defined in (3.14)–(3.17).

Proof. First, we write

$$|a_{11}^n(\theta_h)a_{22}^n(\theta_h) - a_{12}^n(\theta_h)a_{21}^n(\theta_h)|$$

(4.9)
$$= \left[h(S^n(\theta_h) - \beta^n C^n(\theta_h))^T(\mathbf{I} + \mathbf{K}_{\theta_h}^n)(S^n(\theta_h) - \beta^n C^n(\theta_h))\right]$$
$$\times \left[hC^n(\theta_h)^T(\mathbf{I} + \mathbf{K}_{\theta_h}^n)C^n(\theta_h)\right],$$

where

$$\beta^n \equiv \frac{S^n(\theta_h)^T(\mathbf{I} + \mathbf{K}_{\theta_h}^n)C^n(\theta_h)}{C^n(\theta_h)^T(\mathbf{I} + \mathbf{K}_{\theta_h}^n)C^n(\theta_h)}.$$

Using the fact that $\mathbf{I} + \mathbf{K}_{\theta_h}^n \geq 1/2$ for any $h > 0$, we find that

$$
h(S^n(\theta_h) - \beta^n C^n(\theta_h))^T (\mathbf{I} + \mathbf{K}_{\theta_h}^n)(S^n(\theta_h) - \beta^n C^n(\theta_h))
$$

(4.10)
$$
\geq \frac{h}{2}(S^n(\theta_h) - \beta^n C^n(\theta_h))^T (S^n(\theta_h) - \beta^n C^n(\theta_h)),
$$

(4.11)
$$
hC^n(\theta_h)^T (\mathbf{I} + \mathbf{K}_{\theta_h}^n) C^n(\theta_h) \geq \frac{h}{2} C^n(\theta_h)^T C^n(\theta_h).
$$

Next, we observe that for $1 \leq j \leq N$,

$$
S^n(\theta_j) - \beta^n C^n(\theta_j) = -\sqrt{1 + (\beta^n)^2} \frac{\cos(\theta_j^{n+1} - \hat{\theta}^n) - \cos(\theta_j^{n-1} - \hat{\theta}^n)}{\theta_j^{n+1} - \theta_j^{n-1}},
$$

$$
C^n(\theta_j) = -\frac{\cos(\theta_j^{n+1} - \frac{\pi}{2}) - \cos(\theta_j^{n-1} - \frac{\pi}{2})}{\theta_j^{n+1} - \theta_j^{n-1}},
$$

in which

$$
\hat{\theta}^n \equiv \arcsin \frac{\beta^n}{\sqrt{1 + (\beta^n)^2}}.
$$

It follows that

$$
h(S^n(\theta_h) - \beta^n C^n(\theta_h))^T (S^n(\theta_h) - \beta^n C^n(\theta_h))
$$
$$
\geq h \sum_{j=1}^{N} \left[\frac{\cos(\theta_j^{n+1} - \hat{\theta}^n) - \cos(\theta_j^{n-1} - \hat{\theta}^n)}{\theta_j^{n+1} - \theta_j^{n-1}} \right]^2,
$$

$$
hC^n(\theta_h)^T C^n(\theta_h) \geq h \sum_{j=1}^{N} \left[\frac{\cos(\theta_j^{n+1} - \frac{\pi}{2}) - \cos(\theta_j^{n-1} - \frac{\pi}{2})}{\theta_j^{n+1} - \theta_j^{n-1}} \right]^2.
$$

Therefore, the conclusion of the lemma is a consequence of Lemma 4, (4.9), (4.10), and (4.11).

Finally, we state some estimates for $\mathbf{A}^n(\theta_h)$, which is defined in (3.9) with $\mathbf{B}^n(\theta_h)$ given by (3.8), and $\hat{f}^n$, $\hat{g}^n$ determined by the system (3.20) and (3.21). The proofs of these estimates employ standard methods but are quite technical, and the interested reader can find the details in [8]. We suppose throughout that θ_h satisfies Hypothesis (H). Then

(4.12)
$$
\|\mathbf{B}^n(\theta_h)\|_\infty \leq (1 + \|D_h^- \theta_h^{n+1}\|_0^2 + |\theta_h^n|_e^2 + |\theta_h^{n-1}|_e^2),
$$

(4.13)
$$
|\hat{f}^n| \leq C(1 + |\theta_h^n|_e^2 + |\theta_h^{n-1}|_e^2)^2 (1 + \|D_h^- \theta_h^{n+1}\|_0^2 + |\theta_h^n|_e^2 + |\theta_h^{n-1}|_e^2),
$$

(4.14)
$$
|\hat{g}^n| \leq C(1 + |\theta_h^n|_e^2 + |\theta_h^{n-1}|_e^2)^2 (1 + \|D_h^- \theta_h^{n+1}\|_0^2 + |\theta_h^n|_e^2 + |\theta_h^{n-1}|_e^2),
$$

(4.15)
$$
\|\mathbf{A}^n(\theta_h)\|_\infty \leq C(1 + |\theta_h^n|_e^2 + |\theta_h^{n-1}|_e^2)^2
$$
$$
\times (1 + \|D_h^- \theta_h^{n+1}\|_0^2 + |\theta_h^n|_e^2 + |\theta_h^{n-1}|_e^2),
$$

(4.16) $\quad \|(\mathbf{I} + \mathbf{K}_{\theta_h}^n)\mathbf{A}^n(\theta_h)\|_\infty \le C(1 + |\theta_h^n|_e^2 + |\theta_h^{n-1}|_e^2)^2$
$$\times (1 + \|D_h^- \theta_h^{n+1}\|_0^2 + |\theta_h^n|_e^2 + |\theta_h^{n-1}|_e^2),$$

in which $\|\cdot\|_\infty$, $\|\cdot\|_0$, and $|\cdot|_e$ are defined at the end of §1. Furthermore, if φ_h is another mesh function satisfying Hypothesis (H), then

$$\|\mathbf{A}^n(\theta_h) - \mathbf{A}^n(\varphi_h)\|_\infty$$
$$\le C(1 + |\theta_h^n|_e^2 + |\theta_h^{n-1}|_e^2)^2(1 + |\varphi_h^n|_e^2 + |\varphi_h^{n-1}|_e^2)^2$$
(4.17) $\quad \times(1 + \|D_h^- \theta_h^{n+1}\|_0^2 + \|D_h^- \varphi_h^{n+1}\|_0^2 + |\theta_h^n|_e^2 + |\varphi_h^n|_e^2 + |\theta_h^{n-1}|_e^2 + |\varphi_h^{n-1}|_e^2)$
$$\times(\|\theta_h^{n+1} - \varphi_h^{n+1}\|_0 + \|D_h^- \theta_h^{n+1} - D_h^- \varphi_h^{n+1}\|_0$$
$$+ \|\theta_h^n - \varphi_h^n\|_e + \|\theta_h^{n-1} - \varphi_h^{n-1}\|_e)$$

and

$$\|(\mathbf{I} + \mathbf{K}_{\theta_h}^n)\mathbf{A}^n(\theta_h) - (\mathbf{I} + \mathbf{K}_{\varphi_h}^n)\mathbf{A}^n(\varphi_h)\|_\infty$$
$$\le C(1 + |\theta_h^n|_e^2 + |\theta_h^{n-1}|_e^2)^2(1 + |\varphi_h^n|_e^2 + |\varphi_h^{n-1}|_e^2)^2$$
(4.18) $\quad \times(1 + \|D_h^- \theta_h^{n+1}\|_0^2 + \|D_h^- \varphi_h^{n+1}\|_0^2 + |\theta_h^n|_e^2 + |\varphi_h^n|_e^2 + |\theta_h^{n-1}|_e^2 + |\varphi_h^{n-1}|_e^2)$
$$\times(\|\theta_h^{n+1} - \varphi_h^{n+1}\|_0 + \|D_h^- \theta_h^{n+1} - D_h^- \varphi_h^{n+1}\|_0$$
$$+ \|\theta_h^n - \varphi_h^n\|_e + \|\theta_h^{n-1} - \varphi_h^{n-1}\|_e).$$

5. Existence of the discrete solution. We next present an iteration scheme for determining the approximate solution. The convergence of this scheme proves the existence of this solution.

THEOREM 2. *Let φ_h and ψ_h be the mesh functions given by Lemma 2. Then, there exists a $\delta > 0$ such that for $0 < \tau \le \delta$, equation (3.11) subject to (1.15) has a unique solution for $n \ge 1$.*

Proof. The proof is by a standard iteration argument. Setting

$$G^n(\theta_h^{n+1}, \theta_h^n, \theta_h^{n-1})_h = (\mathbf{I} + \mathbf{K}_{\theta_h}^n)\mathbf{A}^n(\theta_h),$$

$$N_{n+1,k} = \|D_h^- \theta_h^{n+1,k}\|_0 + \|\frac{1}{\tau}(\theta_h^{n+1,k} - \theta_h^n)\|_0,$$

and

$$d(\theta_h^{n+1,k}, \varphi_h^{n+1,k}) = \|D_h^- \theta_h^{n+1,k} - D_h^- \varphi_h^{n+1,k}\|_0$$
$$+ \left\|\frac{1}{\tau}(\theta_h^{n+1,k} - \theta_h^n) - \frac{1}{\tau}(\varphi_h^{n+1,k} - \varphi_h^n)\right\|_0 + \|\theta_h^{n+1,k} - \varphi_h^{n+1,k}\|_0,$$

we define the iteration

$$\frac{1}{\tau^2}(\theta_h^{n+1,k+1} - 2\theta_h^n + \theta_h^{n-1}) - D_h^2 \theta_h^n = G^n(\theta_h^{n+1,k}, \theta_h^n, \theta_h^{n-1})_h,$$
$$\theta_h^{n+1,0} = 2\theta_h^n - \theta_h^{n-1}.$$

It is then possible to show that there exists a $\delta > 0$, which depends on the initial data and on the third- and fourth-order derivatives of the exact solution in a neighborhood of $t = 0$ as required by Lemma 2, such that for $0 < \tau \le \delta$,

(i) $\{N_{n+1,k}\}$ is uniformly bounded, and

(ii) $\{d(\theta_h^{n+1,k}, \theta_h^{n+1,k-1})\}$ decreases with a geometric rate. The details of this are quite technical and again we refer the reader to [8]. The uniqueness is a consequence of the fact that any solution of (3.11) conserves discrete energy, and hence, it satisfies Hypothesis (H) and estimates (4.12)–(4.18). Thus, if θ_h and φ_h are two solutions of (3.11), we can employ a similar argument as used in proving the geometric rate decrease of the sequence $\{d(\theta_h^{n,k}, \theta_h^{n,k-1})\}$ to show that for $0 < \tau < \delta$,

$$d(\theta_h^n, \varphi_h^n) \leq \frac{1}{2} d(\theta_h^n, \varphi_h^n) \qquad \text{for } n = 2, 3, \ldots.$$

6. Error estimate. To obtain an error estimate for our approximation scheme, we first estimate the local truncation error of the scheme.

LEMMA 6. *Assume that $\tilde{\theta}$, $\tilde{f}$, and $\tilde{g}$, the exact solution of IBVP (1.1)–(1.7), are in $C^4([0,1] \times [0,T])$ for some $T > 0$. Then, for $(1+n)\tau \leq T$, we have*

$$\triangle_\tau^2 \tilde{\theta}_h^n - D_h^2 \tilde{\theta}_h^n = (\mathbf{I} + \mathbf{K}_{\tilde{\theta}_h}^n) \mathbf{A}^n(\tilde{\theta}_h) + O(\tau^2).$$

Proof. We first show that for $1 \leq j \leq N$,

(6.1)
$$\frac{\cos \tilde{\theta}_j^{n+1} - \cos \tilde{\theta}_j^{n-1}}{\tilde{\theta}_j^{n+1} - \tilde{\theta}_j^{n-1}} = -\sin \tilde{\theta}_j^n + O(\tau^2),$$

(6.2)
$$\frac{\sin \tilde{\theta}_j^{n+1} - \sin \tilde{\theta}_j^{n-1}}{\tilde{\theta}_j^{n+1} - \tilde{\theta}_j^{n-1}} = \cos \tilde{\theta}_j^n + O(\tau^2).$$

Applying the Taylor series expansions, we have

$$\cos \tilde{\theta}_j^{n+1} = \cos \tilde{\theta}_j^n - \sin \tilde{\theta}_j^n (\tilde{\theta}_j^{n+1} - \tilde{\theta}_j^n) - \frac{1}{2} \cos \tilde{\theta}_j^n (\tilde{\theta}_j^{n+1} - \tilde{\theta}_j^n)^2 + \frac{1}{6} \sin \tilde{\theta}_j^n (\tilde{\theta}_j^{n+1} - \tilde{\theta}_j^n)^3 + \cdots,$$

$$\cos \tilde{\theta}_j^{n-1} = \cos \tilde{\theta}_j^n - \sin \tilde{\theta}_j^n (\tilde{\theta}_j^{n-1} - \tilde{\theta}_j^n) - \frac{1}{2} \cos \tilde{\theta}_j^n (\tilde{\theta}_j^{n-1} - \tilde{\theta}_j^n)^2 + \frac{1}{6} \sin \tilde{\theta}_j^n (\tilde{\theta}_j^{n-1} - \tilde{\theta}_j^n)^3 + \cdots.$$

It follows that

$$\cos \tilde{\theta}_j^{n+1} - \cos \tilde{\theta}_j^{n-1} = -\sin \tilde{\theta}_j^n (\tilde{\theta}_j^{n+1} - \tilde{\theta}_j^{n-1})$$
$$- \frac{1}{2} \cos \tilde{\theta}_j^n (\tilde{\theta}_j^{n+1} - \tilde{\theta}_j^{n-1})(\tilde{\theta}_j^{n+1} - 2\tilde{\theta}_j^n + \tilde{\theta}_j^{n-1}) + (\tilde{\theta}_j^{n+1} - \tilde{\theta}_j^{n-1})O(\tau^2).$$

We then use the estimate $\tilde{\theta}_j^{n+1} - 2\tilde{\theta}_j^n + \tilde{\theta}_j^{n-1} = O(\tau^2)$ to obtain formula (6.1). (6.2) can be proven in the same way.

Next, since $\tilde{\theta}$, $\tilde{f}$, and $\tilde{g}$ are in $C^4([0,1] \times [0,T])$, it follows from the system (1.1)–(1.3) that the following relations hold:

$$\tilde{\theta}_{ss}(0,t) = \tilde{\theta}_{ss}(1,t), \quad \tilde{\theta}_{sss}(0,t) = \tilde{\theta}_{sss}(1,t),$$
$$\tilde{f}_{ss}(0,t) = \tilde{f}_{ss}(1,t), \quad \tilde{f}_{sss}(0,t) = \tilde{f}_{sss}(1,t),$$
$$\tilde{g}_{ss}(0,t) = \tilde{g}_{ss}(1,t), \quad \tilde{g}_{sss}(0,t) = \tilde{g}_{sss}(1,t).$$

Hence, applying the Taylor series expansions at $1 \leq j \leq N$, and using (6.1), (6.2), we find that the truncation error for the system (1.1)–(1.3) is of order τ^2 after discretization. Following the procedure given in §3, and noticing that $|K_{ij}| \leq 1$, for $0 \leq i,j \leq N$, we obtain the equation

$$(\mathbf{I} + \mathbf{L}_{\tilde{\theta}_h}^n)(\triangle_\tau^2 \tilde{\theta}_h^n - D_h^2 \tilde{\theta}_h^n) = \mathbf{A}^n(\tilde{\theta}_h) + O(\tau^2).$$

The conclusion of the lemma then follows from the estimate $\|\mathbf{I} + \mathbf{K}^n_{\hat{\theta}_h}\|_\infty \le 2$.

LEMMA 7 (discrete Gronwall inequality). *Let $\{u_n\}$ be a nonnegative sequence. If for $n \ge 1$,*

$$u_n \le A + B \sum_{k=1}^n u_k,$$

where A, $B \ge 0$ and $B < 1$, then for $n \ge 1$,

$$u_n \le \frac{A}{1-B} + \frac{AB}{(1-B)^2} \sum_{k=1}^{n-1} e^{(n-k)\frac{B}{1-B}}.$$

Using these results, we now obtain an error estimate for our approximation scheme.

THEOREM 3. *Let φ_h and ψ_h be the mesh functions given by Lemma 2. Let θ_h denote the solution of equation (3.11) subject to (1.15) and denote by $\hat{\theta}$, $\hat{f}$, and $\hat{g}$ the exact solution. Then, for τ sufficiently small, on any interval $[0,T]$ in which $\hat{\theta}$, $\hat{f}$, and $\hat{g} \in C^4([0,1] \times [0,T])$, with $(n+1)\tau = T$, $h = \sqrt{2}\tau$, there exists a constant C_T, depending on the initial data, on the third and fourth derivatives of the exact solution, and on T, such that*

$$\|\theta^n_h - \hat{\theta}^n_h\|_e \le C_T \tau^2.$$

Proof. To make the notation simple, we denote

$$G^n_h(\theta_h) = (\mathbf{I} + \mathbf{K}^n_{\theta_h})\mathbf{A}^n(\theta_h)$$

and write

$$\triangle^2_\tau \tilde{\theta}^n_h - D^2_h \tilde{\theta}^n_h = G^n_h(\tilde{\theta}_h) + \tau^n_h,$$

where τ^n_h is the truncation error, which is of order τ^2 as shown in Lemma 6. We also introduce $\psi^n_h = \theta^n_h - \tilde{\theta}^n_h$ and define

$$e^n_{\psi_h} = \left(\frac{1}{2} h \sum_{j=1}^N (\triangle^+_\tau \psi^n_j)^2 + \frac{1}{2} h \sum_{j=1}^N (\tilde{D}^-_h \psi^{n+1}_j)(\tilde{D}^-_h \psi^n_j) \right)^{\frac{1}{2}},$$

in which $\tilde{D}^-_h$ is defined by (1.18). It is clear that $\tilde{D}^-_h \psi^n_h = D^-_h \theta^n_h - D^-_h \tilde{\theta}^n_h$ and $\triangle^+_\tau \psi^n_h = \triangle^+_\tau \theta^n_h - \triangle^+_\tau \tilde{\theta}^n_h$. Using an argument similar to that used in proving Lemma 1, part (ii) and (iii), we can obtain the identity

$$(e^n_{\psi_h})^2 = \frac{1}{4} h \sum_{j=1}^N (\triangle^+_\tau \psi^n_j)^2 + \frac{1}{4}\frac{1}{h} \sum_{j=2}^N \left[(\psi^{n+1}_{j-1} - \psi^n_j)^2 + (\psi^{n+1}_j - \psi^n_{j-1})^2 \right]$$
$$+ \frac{1}{4}\frac{1}{h}(\psi^{n+1}_N - \psi^n_1)^2 + \frac{1}{4}\frac{1}{h}(\psi^{n+1}_1 - \psi^n_N)^2,$$

and the estimate

(6.3) $$\|\tilde{D}^-_h \psi^{n+1}_h\|^2_0 + \|\triangle^+_\tau \psi^n_h\|^2_0 + \|\tilde{D}^-_h \psi^n_h\|^2_0 \le 24(e^n_{\psi_h})^2.$$

Proceeding with the error estimate, we find that ψ_h satisfies the following equations:

for $j = 1$,

$$\frac{1}{\tau^2}(\psi_1^{n+1} - 2\psi_1^n + \psi_1^{n-1}) - \frac{1}{h^2}(\psi_2^n - 2\psi_1^n + \psi_N^n) = (G_1^n(\theta_h) - G_1^n(\tilde{\theta}_h)) - \tau_1^n;$$

for $2 \le j \le N - 1$,

$$\frac{1}{\tau^2}(\psi_j^{n+1} - 2\psi_j^n - \psi_j^{n-1}) - \frac{1}{h^2}(\psi_{j+1}^n - 2\psi_j^n - \psi_{j-1}^n) = (G_j^n(\theta_h) - G_j^n(\tilde{\theta}_h)) - \tau_j^n;$$

and for $j = N$,

$$\frac{1}{\tau^2}(\psi_N^{n+1} - 2\psi_N^n + \psi_N^{n-1}) - \frac{1}{h^2}(\psi_1^n - 2\psi_N^n + \psi_{N-1}^n) = (G_N^n(\theta_h) - G_N^n(\hat{\theta}_h)) - \tau_N^n.$$

We multiply the jth equation by $h(\psi_j^{n+1} - \psi_j^{n-1})$, $1 \le j \le N$, and sum j from 1 to N to obtain for $n \ge 1$,

$$(e_{\psi_h}^n)^2 - (e_{\psi_h}^{n-1})^2 = h\sum_{j=1}^N (G_j^n(\theta_h) - G_j^n(\tilde{\theta}_h))(\psi_j^{n+1} - \psi_j^{n-1}) - h\sum_{j=1}^N \tau_j^n(\psi_j^{n+1} - \psi_j^{n-1}).$$

Hence, it follows that

$$(e_{\psi_h}^n)^2 - (e_{\psi_h}^{n-1})^2 \le \tau\big(\|G_h^n(\theta_h) - G_h^n(\tilde{\theta}_h)\|_\infty + \|\tau_h^n\|_\infty\big)\big(\|\triangle_\tau^+\psi_h^n\|_0 + \|\triangle_\tau^+\psi_h^{n-1}\|_0\big).$$

Using the inequality $\|\triangle_\tau^+\psi_h^n\|_0 \le 4e_{\psi_h}^n$ for $n \ge 0$, and cancelling $e_{\psi_h}^n + e_{\psi_h}^{n-1}$ on both sides, we find that for $n \ge 1$,

$$e_{\psi_h}^n - e_{\psi_h}^{n-1} \le 4\tau\big(\|G_h^n(\theta_h) - G_h^n(\tilde{\theta}_h)\|_\infty + \|\tau_h^n\|_\infty\big).$$

Therefore, we get for $n \ge 1$,

(6.4) $$e_{\psi_h}^n \le e_{\psi_h}^0 + 4\tau\sum_{k=1}^n \|\tau_h^k\|_\infty + 4\tau\sum_{k=1}^n \|G_h^k(\theta_h) - G_h^k(\tilde{\theta}_h)\|_\infty.$$

Now, estimate (4.18) implies that for $k \ge 1$,

(6.5)
$$\|G_h^k(\theta_h) - G_h^k(\tilde{\theta}_h)\|_\infty$$
$$\le C_{\theta_h,\tilde{\theta}_h}^k(\|\psi_h^{k+1}\|_0 + \|\tilde{D}_h^-\psi_h^{k+1}\|_0 + \|\psi_h^k\|_0 + \|\triangle_\tau^+\psi_h^k\|_0$$
$$+ \|\tilde{D}_h^-\psi_h^k\|_0 + \|\psi_h^{k-1}\|_0 + \|\triangle_\tau^+\psi_h^{k-1}\|_0 + \|\tilde{D}_h^-\psi_h^{k-1}\|_0),$$

where

$$C_{\theta_h,\tilde{\theta}_h}^k = C(1 + |\theta_h^k|_e^2 + |\theta_h^{k-1}|_e^2)^2(1 + |\tilde{\theta}_h^k|_e^2 + |\tilde{\theta}_h^{k-1}|_e^2)^2$$
$$\times(1 + \|D_h^-\theta_h^{k+1}\|_0^2 + \|D_h^-\tilde{\theta}_h^{k+1}\|_0^2 + |\theta_h^k|_e^2 + |\tilde{\theta}_h^k|_e^2 + |\theta_h^{k-1}|_e^2 + |\tilde{\theta}_h^{k-1}|_e^2).$$

Conservation of the discrete energy and conservation of the total energy for the continuous system imply that there exists a constant $\delta > 0$ and a constant $C > 0$ such that for $0 < \tau \le \delta$, if $(k+1)\tau \le T$, then

$$C_{\theta_h,\tilde{\theta}_h}^k \le C.$$

Hence, putting (6.5) into (6.4), using Lemma 1 (iii), and rearranging the summation, we obtain that for $n \geq 1$,

$$(6.6) \qquad e_{\psi_h}^n \leq \bar{\gamma}_0 + \tau C \sum_{k=1}^n (\|\psi_h^{k+1}\|_0 + e_{\psi_h}^k),$$

in which

$$\bar{\gamma}_0 = C \left(\|\psi_h^0\|_0 + \|\tilde{D}_h^- \psi_h^0\|_0 + \|\triangle_\tau^+ \psi_h^0\|_0 + \|\psi_h^1\|_0 + \|\tilde{D}_h^- \psi_h^1\|_0 + \tau \sum_{k=1}^n \|\tau_h^k\|_\infty \right).$$

To estimate $\|\psi_h^{n+1}\|_0$, we rewrite the equations for ψ_h as follows: for $j = 1$,

$$\psi_1^{n+1} = \frac{1}{2}\psi_2^n + \frac{1}{2}\psi_N^n + (\psi_1^n - \psi_1^{n-1}) + \tau^2(G_1^n(\theta_h) - G_1^n(\tilde{\theta}_h)) - \tau^2 \tau_1^n;$$

for $2 \leq j \leq N - 1$,

$$\psi_j^{n+1} = \frac{1}{2}\psi_{j+1}^n + \frac{1}{2}\psi_{j-1}^n + (\psi_j^n - \psi_j^{n-1}) + \tau^2(G_j^n(\theta_h) - G_j^n(\tilde{\theta}_h)) - \tau^2 \tau_j^n;$$

and for $j = N$,

$$\psi_N^{n+1} = \frac{1}{2}\psi_1^n + \frac{1}{2}\psi_{N-1}^n + (\psi_N^n - \psi_N^{n-1}) + \tau^2(G_N^n(\theta_h) - G_N^n(\tilde{\theta}_h)) - \tau^2 \tau_N^n.$$

Multiply the jth equation by $h\psi_j^{n+1}$, $1 \leq j \leq N$, and sum j from 1 to N to obtain

$$\begin{aligned}
h \sum_{j=1}^N (\psi_j^{n+1})^2 = {} & \frac{1}{2} \left(h\psi_2^n \psi_1^{n+1} + h \sum_{j=2}^{N-1} \psi_{j+1}^n \psi_j^{n+1} + h\psi_1^n \psi_N^{n+1} \right) \\
& + \frac{1}{2} \left(h\psi_N^n \psi_1^{n+1} + h \sum_{j=2}^{N-1} \psi_{j-1}^n \psi_j^{n+1} + h\psi_{N-1}^n \psi_N^{n+1} \right) \\
& + h \sum_{j=1}^N (\psi_j^n - \psi_j^{n-1})\psi_j^{n+1} + \tau^2 \sum_{j=1}^N (G_j^n(\theta_h) - G_j^n(\tilde{\theta}_h))\psi_j^{n+1} \\
& - \tau^2 h \sum_{j=1}^N \tau_j^n \psi_j^{n+1}.
\end{aligned}$$

Applying the Cauchy–Schwarz inequality to the right side and cancelling $\|\psi_h^{n+1}\|_0$ on both sides, we obtain for $n \geq 1$,

$$\|\psi_h^{n+1}\|_0 - \|\psi_h^n\|_0 \leq \tau\|\triangle_\tau^+ \psi_h^{n-1}\|_0 + \tau^2\|G_h^n(\theta_h) - G_h^n(\tilde{\theta}_h)\|_\infty + \tau^2\|\tau_h^n\|_\infty.$$

Hence, it follows that

$$\begin{aligned}
\|\psi_h^{n+1}\|_0 \leq {} & \left(\|\psi_h^1\|_0 + \|\triangle_\tau^+ \psi_h^0\|_0 + \tau \sum_{k=1}^n \|\tau_h^k\|_\infty \right) + \tau \sum_{k=1}^{n-1} \|\triangle_\tau^+ \psi_h^k\|_0 \\
& + \tau^2 \sum_{k=1}^n \|G_h^k(\theta_h) - G_h^k(\tilde{\theta}_h)\|_\infty.
\end{aligned}$$

Again, using (6.5), Lemma 1 (iii), and rearranging the summation, we find that for $n \geq 1$,

$$(6.7) \qquad \|\psi_h^{n+1}\|_0 \leq \tilde{\gamma}_0 + \tau C \sum_{k=1}^{n} (\|\psi_h^{k+1}\|_0 + e_{\psi_h}^k),$$

in which

$$\tilde{\gamma}_0 = C \left(\|\psi_h^0\|_0 + \|\tilde{D}_h^- \psi_h^0\|_0 + \|\triangle_\tau^+ \psi_h^0\|_0 + \|\psi_h^1\|_0 + \|\tilde{D}_h^- \psi_h^1\|_0 + \tau \sum_{k=1}^{n} \|\tau_h^k\|_\infty \right)$$

Combine (6.6) and (6.7) to obtain for $n \geq 1$,

$$\|\psi_h^{n+1}\|_0 + e_{\psi_h}^n \leq \gamma_0 + \tau C \sum_{k=1}^{n} (\|\psi_h^{k+1}\|_0 + e_{\psi_h}^k),$$

where

$$\gamma_0 = C \left(\|\psi_h^0\|_0 + \|\tilde{D}_h^- \psi_h^0\|_0 + \|\triangle_\tau^+ \psi_h^0\|_0 + \|\psi_h^1\|_0 + \|\tilde{D}_h^- \psi_h^1\|_0 + \tau \sum_{k=1}^{n} \|\tau_h^k\|_\infty \right).$$

For τ sufficiently small such that $\tau C \leq 1/2$, the discrete Gronwall inequality implies that for $n \geq 1$,

$$\|\psi_h^{n+1}\|_0 + e_{\psi_h}^n \leq C\gamma_0.$$

From Lemmas 2 and 6, it is clear that γ_0 is of order τ^2. Using estimate (6.3), the conclusion of the theorem follows.

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