Semidiscrete-Least Squares Methods for a Parabolic Boundary Value Problem*

By James H. Bramble and Vidar Thomée

Abstract. In this paper some approximate methods for solving the initial-boundary value problem for the heat equation in a cylinder under homogeneous boundary conditions are analyzed. The methods consist in discretizing with respect to time and solving approximately the resulting elliptic problem for fixed time by least squares methods. The approximate solutions will belong to a finite-dimensional subspace of functions in space which will not be required to satisfy the homogeneous boundary conditions.

1. Introduction. The purpose of this paper is to analyze some approximate methods for solving the initial-boundary value problem for the heat equation in a cylinder under homogeneous boundary conditions. The methods consist in discretizing with respect to time and solving approximately the resulting elliptic problem for fixed time by least squares methods. The approximate solutions will belong to a finite-dimensional subspace of functions in space which will not be required to satisfy the homogeneous boundary conditions.

Let Ω be a bounded domain in Euclidean N-space R^N with smooth boundary $\partial \Omega$. We shall consider the approximate solution of the following mixed initial-boundary value problem for u = u(x, t), namely,

(1.1)
$$\frac{\partial u}{\partial t} = \Delta u \equiv \sum_{i=1}^{N} \frac{\partial^{2} u}{\partial x_{i}^{2}} \quad \text{in } \Omega \times (0, \infty),$$

$$u = 0 \quad \text{on } \partial \Omega \times [0, \infty),$$

$$u(x, 0) = v(x) \quad \text{in } \Omega.$$

By replacing the time derivative in (1.1) by a backward-difference quotient, we define an approximate solution $u_k(x, t)$ for t = nk, $n = 0, 1, 2, \dots$, by

(1.2)
$$\frac{u_k(x, t+k) - u_k(x, t)}{k} = \Delta u_k(x, t+k), \qquad x \in \Omega,$$
$$u_k = 0, \qquad x \in \partial \Omega,$$
$$u_k(x, 0) = v(x), \qquad x \in \Omega.$$

With $u_k(x, t) = v$, $u_k(x, t + k) = w$, we then have the following equation to solve for w, when v is known:

$$(1.3) w - k\Delta w = v in \Omega,$$

$$(1.4) w = 0 on \partial \Omega.$$

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We shall prove that this Dirichlet problem admits a unique solution and that, for sufficiently smooth initial-values v,

$$\sup_{0 \le t \le T} ||u_k(\cdot, t) - u(\cdot, t)|| = O(k) \quad \text{as } k \to 0,$$

where $||\cdot||$ denotes the norm in $L_2(\Omega)$,

$$||v|| = \left(\int_{0}^{\infty} |v(x)|^{2} dx\right)^{1/2}.$$

For the approximate solution of the problem (1.3), (1.4), we shall use a finite-dimensional subspace S_h^{μ} depending on a small positive parameter h such that for any v in $H^{\mu+2}$, $\mu \ge 0$ (or in a certain subspace of $H^{\mu+2}$), there is a $\varphi \in S_h^{\mu}$ such that

$$||v - \varphi||_{H^{j}} \le Ch^{2+\mu-j}||v||_{H^{\mu+2}}, \quad 0 \le j \le 2.$$

Here, $H^i = W_2^i(\Omega)$, $j = 0, 1, 2, \cdots$, denotes the Sobolev space defined by

$$||v||_{H^i} = \sum_{|\alpha| \leq i} ||D^{\alpha}v||.$$

The functions in S_h^{μ} are not assumed to satisfy the homogeneous boundary conditions on $\partial\Omega$.

Given v, we shall then take for the approximate solution of (1.3), (1.4) the unique function in S_h^{μ} which minimizes the functional

(1.5)
$$\Lambda(\varphi;v) = ||\varphi - k\Delta\varphi - v||^2 + \gamma_{kh}|\varphi|^2,$$

where $|\cdot|$ denotes the norm on $L_2(\partial\Omega)$,

$$|v| = \left(\int_{\partial\Omega} |v(x)|^2 dS\right)^{1/2}.$$

The selection of the weight γ_{kh} in (1.5) is crucial and depends upon an a priori inequality for the elliptic operator in (1.3). It will turn out that it is appropriate to choose γ_{kh} such that, for certain positive γ and C,

$$\gamma k^{1/2} \leq \gamma_{kh} \leq Ck^2 h^{-3}.$$

If we thus define $u_{kh}(x, t)$, t = nk, $n = 0, 1, 2, \dots$, by setting

$$\Lambda(u_{kh}(\cdot, t + k); u_{kh}(\cdot, t)) = \min_{\varphi \in Sh^{\mu}} \Lambda(\varphi; u_{kh}(\cdot, t)),$$

$$u_{kh}(x, 0) = v(x), \qquad x \in \Omega,$$

we shall be able to prove that

$$\sup_{0 \le t \le T} ||u_{kh}(\cdot, t) - u(\cdot, t)|| = O(k + h^{\mu}) \text{ as } k, h \to 0.$$

Notice here that (1.6) implies that kh^{-2} is bounded away from zero. This requirement goes in the opposite direction compared to the well-known stability requirement for explicit difference schemes. Notice also that as a consequence of this requirement the error estimate has the form O(k) for all $\mu \ge 2$.

In order to obtain greater accuracy, it is natural to consider, instead of (1.2), the Crank-Nicolson symmetric formula

$$\frac{\ddot{u}_{k}(x, t + k) - \ddot{u}_{k}(x, t)}{k} = \frac{1}{2} \Delta \ddot{u}_{k}(x, t + k) + \frac{1}{2} \Delta \ddot{u}_{k}(x, t).$$

In this case, the problem (1.3), (1.4) changes into

$$(1.7) w - \frac{1}{2}k\Delta w = v + \frac{1}{2}k\Delta v \text{ in } \Omega,$$

$$(1.8) w = 0 on \partial \Omega.$$

This problem again admits a unique solution and we shall now prove a convergence result which this time takes the form

$$\sup_{0 \le t \le T} ||\tilde{u}_k(\cdot, t) - u(\cdot, t)|| = O(k^2) \quad \text{as } k \to 0.$$

In order to solve the problem (1.7), (1.8) approximately, we shall introduce the functional

$$\tilde{\Lambda}(\varphi;v) = ||\varphi - \frac{1}{2}k\Delta\varphi - v - \frac{1}{2}k\Delta v||^2 + \tilde{\gamma}_{kh}|\varphi|^2,$$

where now the weight $\tilde{\gamma}_{kh}$ will be chosen to satisfy

$$\gamma_{\alpha} \leq \tilde{\gamma}_{kh} \leq Ck^2h^{-3},$$

with positive γ_{α} and C. With the appropriate definition of \tilde{u}_{kh} , we shall then prove

$$\sup_{0 \le t \le T} ||\tilde{u}_{kh}(\cdot, t) - u(\cdot, t)|| = O(k^2 + h^{\mu}) \text{ as } k, h \to 0.$$

By (1.9), $k^2 \ge ch^3$ and, hence, the error estimate here has the form $O(k^2)$ for all $\mu \ge 3$. All the above convergence estimates require v to be sufficiently smooth. The exact degree of regularity assumed in each case will be clear from the statement of our theorems below. For v less regular, we shall prove correspondingly weaker convergence estimates. In the case of the approximate Crank-Nicolson method, a specific difficulty appears in that the functional $\tilde{\Lambda}$ contains Δv and, thus, requires more regularity from the initial-values than in the purely implicit method. As we shall see, this difficulty can be overcome, for instance, by taking the first step by the purely implicit method.

In the extensive recent literature dealing with the solution of elliptic and parabolic problems by variational methods, many papers concerned with homogeneous boundary conditions employ finite-dimensional subspaces of the relevant Hilbert spaces, the elements of which satisfy the boundary conditions. In the parabolic case, such techniques have been analysed by Price and Varga [14] and Douglas and Dupont [9]. In order to avoid the difficulty of constructing subspaces with a prescribed behavior at the boundary, different variational principles have been considered where, for the approximate solution, the boundary values are assumed only approximately; cf. Aubin [2], Babuška [3], Bramble and Schatz [6]. The method of solution of the elliptic problems above at fixed time is that of Bramble and Schatz. The analysis of the effect of the discretization in time is similar to that in Peetre and Thomée [13]. A somewhat different way of applying the ideas in [6] in parabolic problems has been described in King [11].

2. The Continuous Problem. In this section, we shall prove an a priori estimate for the continuous problem which we shall need for our error estimates. For this purpose we recall some properties of the eigenvalue problem

$$(2.1) \Delta v + \lambda v = 0 in \Omega,$$

$$(2.2) v = 0 on \partial \Omega.$$

We collect what we need in the following lemma.

LEMMA 2.1. The eigenvalue problem (2.1), (2.2) admits a sequence $\{\lambda_m\}_1^{\infty}$ of positive eigenvalues and a corresponding sequence $\{\varphi_m\}_1^{\infty}$ of eigenfunctions which constitute an orthonormal basis in $L_2(\Omega)$; every $v \in L_2(\Omega)$ may be represented as

(2.3)
$$v(x) = \sum_{m=1}^{\infty} \beta_m \varphi_m(x), \qquad \beta_m = ((v, \varphi_m)) = \int_{\Omega} v(x) \varphi_m(x) \ dx$$

and Parseval's relation

$$||v|| = \left(\sum_{m} |\beta_{m}|^{2}\right)^{1/2}$$

holds.

Let \dot{H}^s , with $s \ge 0$, be the subspace of $L_2(\Omega)$ for which

$$||v||_s = \left(\sum_m \lambda_m^s |\beta_m|^2\right)^{1/2} < \infty, \qquad \beta_m = ((v, \varphi_m)),$$

and let $\dot{H}^{\infty} = \bigcap_{s>0} \dot{H}^s$. It is easy to see that, if $\partial \Omega \in \mathfrak{C}^{\infty}$, we have

$$\dot{H}^{\infty} = \{v; v \in \mathfrak{C}^{\infty}(\overline{\Omega}), \, \Delta^{i}v = 0 \text{ on } \partial\Omega, \, j = 0, 1, \, \cdots \},$$

and for s an integer,

$$|c_s||v||_{H^s} \le ||v||_s = ((-\Delta)^s v, v) \le |c_s||v||_{H^s}, \quad v \in \dot{H}^{\infty}.$$

The spaces \dot{H}^s have the following interpolation property (cf., e.g., [12]):

Lemma 2.2. Let $s_0 < s < s_1$. Then, there is a constant C such that, if α is a bounded linear mapping from \dot{H}^{s_i} into a normed linear space $\mathfrak A$ with norm $||\cdot||_{\mathfrak A}$ such that

$$||\alpha v||_{\mathfrak{A}} \leq A_{i}||v||_{s_{i}}, \quad j = 0, 1,$$

then $\mathfrak A$ is also a bounded linear mapping from \dot{H}^s into $\mathfrak A$ and

$$||\Omega v||_{\mathfrak{A}} \leq C A_0^{1-\theta} A_1^{\theta} ||v||_{s}, \qquad \theta = (s - s_0)/(s_1 - s_0).$$

Consider now the initial-value problem

$$\partial u/\partial t = \Delta u \quad \text{in } \Omega \times (0, \infty),$$

$$(2.5) u = 0 on \partial \Omega \times (0, \infty),$$

$$(2.6) u(x, 0) = v(x) in \Omega.$$

THEOREM 2.1. This problem admits for $v \in \dot{H}^{\infty}$ a unique solution u(x, t) = E(t)v. The linear operator thus defined satisfies

$$(2.7) ||E(t)v|| \le ||v||,$$

and hence may be considered defined on all of $L_2(\Omega)$. Furthermore, E(t)v is smooth for t > 0. For any l and s with $0 \le s \le l$, there is a constant C such that $v \in \dot{H}^s$ implies

 $E(t)v \in \dot{H}^{l}$ and

$$(2.8) ||E(t)v||_{l} \leq Ct^{-(l-s)/2}||v||_{s}, t > 0.$$

Proof. For $v \in \dot{H}^{\infty}$ defined by (2.3), set

$$E(t)v = \sum_{m} \beta_{m} e^{-\lambda_{m} t} \varphi_{m}(x).$$

Then u(x, t) = E(t)v is the unique solution of the problem (2.4), (2.5), (2.6) and the inequality (2.7) follows at once by Parseval's relation. Since, for t > 0,

$$\lambda_m^{l-s} e^{-2\lambda_m t} = t^{-(l-s)} (\lambda_m t)^{l-s} e^{-2\lambda_m t} \le C t^{-(l-s)},$$

we obtain

$$\begin{aligned} ||E(t)v||_{l} &= \left(\sum_{m} \lambda_{m}^{l} |\beta_{m}|^{2} e^{-2\lambda_{m} t}\right)^{1/2} \\ &\leq C t^{-(l-s)/2} \left(\sum_{m} \lambda_{m}^{s} |\beta_{m}|^{2}\right)^{1/2} = C t^{-(l-s)/2} ||v||_{s}, \end{aligned}$$

which proves (2.8).

- 3. The Semidiscrete Problems. We shall discuss here the two problems obtained by backward and symmetric discretization with respect to time.
- (a) The Purely Implicit Method. We shall first consider the problem (1.3), (1.4), described in the introduction. More precisely, we introduce the elliptic operator $L_k = I k\Delta$ and let E_k : $v \to w = E_k v$ be defined by the solution of the following Dirichlet problem:

$$(3.1) L_k w = v in \Omega,$$

$$(3.2) w = 0 on \partial \Omega.$$

For t = nk, we then define $E_k(t)v = E_k^n v$. These definitions are justified by the following theorem.

THEOREM 3.1. The semidiscrete problem (3.1), (3.2) admits a unique solution w, and $w = E_k v$ defines a bounded linear operator E_k in $L_2(\Omega)$. If $0 \le s \le l$ and T > 0, then, for $\frac{1}{2}k(l-s) \le t = nk \le T$, $E_k(t) = E_k^n$ is a bounded linear operator from \dot{H}^s into \dot{H}^l and there is a constant C such that, for $v \in \dot{H}^s$,

$$||E_k(t)v||_l \leq Ct^{-(l-s)/2}||v||_s$$
.

Proof. For v of the form (2.3), we have

$$E_k v(x) = \sum_m \frac{1}{1 + k \lambda_m} \beta_m \varphi_m(x).$$

By Parseval's relation, we have at once $||E_k v|| \le ||v||$. Applying the inequality

$$\tau^{(l-s)/2}/(1+\tau/n)^n \le C, \qquad \tau \ge 0, \qquad n \ge \frac{1}{2}(l-s),$$

valid for *l*, *s* fixed, we obtain

$$\lambda_m^l/(1+k\lambda_m)^{2n} \leq C^2(nk)^{-(l-s)}\lambda_m^s,$$

and, hence,

$$||E_{k}^{n}v||_{l} = \left(\sum_{m} \frac{\lambda_{m}^{l}}{(1+k\lambda_{m})^{2n}} |\beta_{m}|^{2}\right)^{1/2} \leq C(nk)^{-(l-s)/2} \left(\sum_{m} \lambda_{m}^{s} |\beta_{m}|^{2}\right)^{1/2}$$
$$= Ct^{-(l-s)/2} ||v||_{s},$$

which proves the theorem.

Our main interest is to analyze the convergence properties, as $k \to 0$, of the operator $E_k(t)$.

LEMMA 3.1. There is a constant C such that, for $\tau \geq 0$,

$$(3.3) |1/(1+\tau)-e^{-\tau}| \leq |1-(1+\tau)e^{-\tau}| \leq C\tau^2,$$

$$(3.4) |1/(1+\tau)^n - e^{-n\tau}| \le C\tau, n = 1, 2, \cdots.$$

Proof. It is clearly sufficient to prove these inequalities for $0 \le \tau \le 1$. The inequality (3.3) is then obvious. To prove (3.4), we notice that, for $0 \le \tau \le 1$,

$$1/(1+\tau) \le e^{-\tau/2}$$

and, hence, using (3.3),

$$\left| \frac{1}{(1+\tau)^n} - e^{-n\tau} \right| = \left| \frac{1}{1+\tau} - e^{-\tau} \right| \sum_{j=0}^{n-1} \frac{1}{(1+\tau)^j} e^{-(n-1-j)\tau}$$

$$\leq Cn\tau^2 e^{-n\tau/2} \leq C\tau.$$

THEOREM 3.2. There is a constant C such that, for $0 \le s \le 2$, $v \in \dot{H}^s$, and $0 \le t = nk \le T$,

$$||E_k(t)v - E(t)v|| \le Ck^{s/2}||v||_s$$

Proof. For v of the form (2.3), we have, for t = nk,

$$||E_k(t)v - E(t)v|| = \left(\sum_m \left|\frac{1}{(1+k\lambda_m)^n} - e^{-nk\lambda_m}\right|^2 |\beta_m|^2\right)^{1/2}.$$

Using (3.4) of Lemma 3.1, we have the validity for s = 2 of

$$|1/(1+k\lambda_m)^n-e^{-nk\lambda_m}|\leq C(k\lambda_m)^{s/2}.$$

Since the inequality obviously also holds for s = 0, it holds for all s with $0 \le s \le 2$. Consequently, we have, for such s,

$$||E_k(t)v - E(t)v|| \le Ck^{s/2} \Big(\sum_m \lambda_m^s |\beta_m|^2\Big)^{1/2} = Ck^{s/2} ||v||_s,$$

which proves the theorem.

For later use, we notice:

LEMMA 3.2. There is a constant C such that, for $0 \le s \le 4$ and $v \in \dot{H}^s$,

$$||E_k v - E(k)v|| \le ||L_k(E_k - E(k))v|| \le Ck^{s/2}||v||_s.$$

Proof. Using the fact that by (3.3) of Lemma 3.1, for $0 \le s \le 4$,

$$\left|\frac{1}{1+k\lambda_m}-e^{-k\lambda_m}\right| \leq |1-(1+k\lambda_m)e^{-k\lambda_m}| \leq C(k\lambda_m)^{s/2},$$

we obtain

$$||E_{k}v - E(k)v|| \leq ||L_{k}(E_{k} - E(k))v||$$

$$= \left(\sum_{m} |1 - e^{-k\lambda_{m}}(1 + k\lambda_{m})|^{2}|\beta_{m}|^{2}\right)^{1/2}$$

$$\leq Ck^{s/2} \left(\sum_{m} \lambda_{m}^{s}|\beta_{m}|^{2}\right)^{1/2} \leq Ck^{s/2}||v||_{s}.$$

(b) The Crank-Nicolson Method. In order to obtain higher accuracy, we shall consider here the operator \tilde{E}_k : $v \to w = \tilde{E}_k v$ corresponding to the symmetric discretization

$$(w - v)/k = \Delta(\frac{1}{2}w + \frac{1}{2}v).$$

Setting $L_k^{\pm} = I \pm \frac{1}{2}k\Delta$, $w = \tilde{E}_k v$ is defined this time as the solution of the Dirichlet problem

$$(3.5) L_k^- w = L_k^+ v in \Omega,$$

$$(3.6) w = 0 on \partial \Omega.$$

We shall then for t = nk consider the semidiscrete solution $\tilde{E}_k(t)v = \tilde{E}_k^n v$ and its convergence, as k tends to zero, to the solution E(t)v of the continuous problem. Although, formally, (3.5) requires that one can apply the Laplacian to the initial-values, we shall see that \tilde{E}_k is bounded in L_2 . We have more precisely the following.

THEOREM 3.3. The semidiscrete problem (3.5), (3.6) has a unique solution w and $w = \tilde{E}_k v$ defines a bounded linear operator in $L_2(\Omega)$. If $s \ge 0$ and $T \ge 0$, we have, for $v \in \dot{H}^s$ and $0 \le t = nk \le T$,

$$||\tilde{E}_k(t)v||_s \leq ||v||_s.$$

Proof. For v of the form (2.3), we have

$$\tilde{E}_k v(x) = \sum_m \frac{1 - \frac{1}{2}k\lambda_m}{1 + \frac{1}{2}k\lambda_m} \beta_m \varphi_m(x),$$

and, by repeated application,

$$||\tilde{E}_{k}(t)v||_{s} = \left(\sum_{m} \lambda_{m}^{s} \left| \left(\frac{1 - \frac{1}{2}k\lambda_{m}}{1 + \frac{1}{2}k\lambda_{m}}\right)^{n} \beta_{m} \right|^{2}\right)^{1/2}$$

$$\leq \left(\sum_{m} \lambda_{m}^{s} |\beta_{m}|^{2}\right)^{1/2} = ||v||_{s}.$$

Notice that $\tilde{E}_k(t)$ does not have the smoothing property that $E_k(t)$ had. LEMMA 3.3. There is a constant C such that, for $\tau > 0$,

(3.7)
$$\left| \frac{1 - \frac{1}{2}\tau}{1 + \frac{1}{2}\tau} - e^{-\tau} \right| \leq (1 + \frac{1}{2}\tau) \left| \frac{1 - \frac{1}{2}\tau}{1 + \frac{1}{2}\tau} - e^{-\tau} \right| \leq C\tau^{3},$$

$$\left| \left(\frac{1 - \frac{1}{2}\tau}{1 + \frac{1}{2}\tau} \right)^{n} - e^{-n\tau} \right| \leq C\tau^{2}, \qquad n = 1, 2, \cdots.$$

Proof. In both cases, it is sufficient to consider $0 \le \tau \le 1$. The first inequalities are then again obvious. We have, for $0 \le \tau \le 1$,

$$(1 - \frac{1}{2}\tau)/(1 + \frac{1}{2}\tau) \le e^{-\tau/2}$$

and, hence,

$$\left| \left(\frac{1 - \frac{1}{2}\tau}{1 + \frac{1}{2}\tau} \right)^{n} - e^{-n\tau} \right| \leq \left| \frac{1 - \frac{1}{2}\tau}{1 + \frac{1}{2}\tau} - e^{-\tau} \right| \sum_{i=0}^{n-1} \left(\frac{1 - \frac{1}{2}\tau}{1 + \frac{1}{2}\tau} \right)^{i} e^{-(n-1-i)\tau}$$
$$\leq Cn\tau^{3} e^{-n\tau/2} \leq C\tau^{2},$$

which proves (3.7).

In the same way as in the proof of Theorem 3.2, application of this lemma gives the following two results.

THEOREM 3.4. There is a constant C such that, for $0 \le s \le 4$, $v \in \dot{H}^s$, and $0 \le t = nk \le T$,

$$||\tilde{E}_k(t)v - E(t)v|| \leq Ck^{s/2}||v||_s.$$

LEMMA 3.4. There is a constant C such that, for $0 \le s \le 6$ and $v \in \dot{H}^s$,

$$||L_k^-(\tilde{E}_k - E(k))v|| \leq Ck^{s/2}||v||_s.$$

4. Some A Priori Estimates. In this section, we collect some a priori estimates which will be crucial for the analysis of the discrete problem. In addition to the norms in $L_2(\Omega)$ and $L_2(\partial\Omega)$, we shall use the corresponding inner products, which we shall denote by $((\cdot, \cdot))$ and (\cdot, \cdot) , respectively. Further, we shall use the Dirichlet integral defined by

$$D(v, w) = \int_{\Omega} \sum_{i=1}^{N} \frac{\partial v}{\partial x_{i}} \frac{\partial w}{\partial x_{i}} dx.$$

LEMMA 4.1. There is a positive constant C such that, for any $\epsilon > 0$ and $v \in H^1$,

$$|v| \leq \epsilon ||v||_{H^1} + C\epsilon^{-1}||v||.$$

Proof. Let $f = (f_1, \dots, f_N) \in \mathfrak{C}^1(\Omega)$ be such that $f = \nu$ on $\partial \Omega$, where ν is the exterior normal of $\partial \Omega$. Using Gauss' formula, we obtain

$$\int_{\partial\Omega} v^2 ds = \int_{\Omega} \sum_{i=1}^{N} \frac{\partial}{\partial x_i} (f_i v^2) dx$$

$$= \int_{\Omega} \operatorname{div} f \cdot v^2 dx + \int_{\Omega} \sum_{i=1}^{N} f_i 2v \frac{\partial v}{\partial x_i} dx,$$

and, hence, the result follows by trivial estimates.

Lemma 4.2. There is a constant C such that for any $v \in H^2$ vanishing on $\partial \Omega$ and any $\epsilon > 0$,

$$\left|\frac{\partial v}{\partial \nu}\right|^2 \leq \epsilon ||\Delta v||^2 + C\epsilon^{-1} D(v, v).$$

Proof. By Lemma 4.1, we have, for any j,

$$\left|\frac{\partial v}{\partial x_i}\right|^2 \leq \epsilon ||v||_{H^2}^2 + C\epsilon^{-1} D(v,v).$$

The result, therefore, follows by the well-known estimate,

$$||v||_{H^2} \leq C||\Delta v||, \quad v = 0 \quad \text{on } \partial\Omega.$$

The following two lemmas are a priori estimates for the elliptic operators involved in the semidiscrete problems treated in Section 3.

LEMMA 4.3. There is a constant γ such that, for $v \in H^2$,

$$||v||^2 \le ||L_k v||^2 + \gamma k^{1/2} |v|^2.$$

Proof. It suffices to prove the inequality for smooth v. Write v = H + w where $\Delta H = 0$ in Ω , w = 0 on $\partial \Omega$. We have

$$||v||^2 - ||L_k v||^2 = 2k((v, \Delta v)) - k^2 ||\Delta v||^2$$

= $2k((v, \Delta w)) - k^2 ||\Delta w||^2$.

Now,

$$((v, \Delta w)) = \left(v, \frac{\partial w}{\partial v}\right) - D(v, w) = \left(v, \frac{\partial w}{\partial v}\right) - D(w, w),$$

since D(H, w) = 0, and hence using Lemma 4.2 with $\epsilon = \gamma k^{1/2}$,

$$2k((v, \Delta w)) \leq \gamma k^{1/2} |v|^2 + k^{3/2} \gamma^{-1} \left| \frac{\partial w}{\partial v} \right|^2 - 2k D(w, w)$$

$$\leq \gamma k^{1/2} |v|^2 + k^2 ||\Delta w||^2 + (C_1 \gamma^{-2} - 2)k D(w, w).$$

The result now follows if we choose $\gamma \ge (\frac{1}{2}C_1)^{1/2}$.

LEMMA 4.4. For any $\alpha > 0$, there is a positive constant γ_{α} such that, for $v \in H^2$,

$$||L_k^+v||^2 \leq (1+\alpha k)(||L_k^-v||^2+\gamma_\alpha |v|^2).$$

Proof. We have as above, with v = H + w,

$$||L_k^+v||^2 - ||L_k^-v||^2 = 2k((v, \Delta v)) = 2k((v, \Delta w)) = 2k\left(v, \frac{\partial w}{\partial v}\right) - 2kD(w, w).$$

Now, by the Cauchy inequality and Lemma 4.2 with $\epsilon = \frac{1}{2}C_1k\beta^{-1}$,

$$2k\left(v,\frac{\partial w}{\partial \nu}\right) \leq \beta |v|^2 + k^2 \beta^{-1} \left|\frac{\partial w}{\partial \nu}\right|^2$$
$$\leq \beta |v|^2 + \frac{1}{2}k^3 C_1 \beta^{-2} ||\Delta w||^2 + 2kD(w,w),$$

or since by Lemma 4.3,

$$(\frac{1}{2}k||\Delta w||)^{2} = (\frac{1}{2}k||\Delta v||)^{2} \le 2||v||^{2} + 2||L_{k}^{-}v||^{2}$$
$$\le 4||L_{k}^{-}v||^{2} + 2\gamma k^{1/2}|v|^{2},$$

we obtain

$$||L_k^+v||^2 - ||L_k^-v||^2 \le 8kC_1\beta^{-2}||L_k^-v||^2 + (\beta + 4\gamma C_1k^{3/2}\beta^{-2})|v|^2.$$

The result now follows if we choose $\beta = (8C_1\alpha^{-1})^{1/2}$.

For later reference, we conclude this section with the following trivial estimate. Lemma 4.5. Let θ , T, and q be positive. Then there is a constant C such that, for $nk \leq T$,

$$k \sum_{j=0}^{n} ((j + \theta)k)^{-q} \le C \left(\log \frac{T}{k}\right)^{\delta_{q,1}} k^{\min(0,1-q)},$$

where $\delta_{q,1}$ is the Kronecker delta.

5. The Discrete Problems. We shall employ for the approximate solution of the semidiscrete problems finite-dimensional subspaces S_h^{μ} of H^2 which approximate H^2 with accuracy μ in the sense that, for $0 \le s \le \mu$, there exists a positive constant C such that, for any $v \in \dot{H}^{2+s}$, there is a $v_h \in S_h^{\mu}$ such that

$$||v-v_h||_{H^l} \leq Ch^{s+2-l}||v||_{s+2}, \qquad l \leq 2.$$

This implies the existence of a positive constant C such that, for $v \in \dot{H}^{2+s}$,

$$\inf_{\varphi \in S_{h^{\mu}}} \sum_{l=0}^{2} h^{l-2} ||v - \varphi||_{H^{1}} \leq Ch^{s} ||v||_{2+s}.$$

Hence, when we refer to the subspace S_h^u , we shall mean any fixed subspace satisfying the above property. Such spaces have been constructed recently by many authors. Typical examples include piecewise polynomial functions such as piecewise Hermite polynomials [5], spline functions or "hill functions" [4], [10], [16], or "triangular elements" [7], [17]. See also [1], [8], [15].

We shall now formulate and analyze the discrete problems.

(a) The Purely Implicit Method. We shall not be able to solve the Dirichlet problem

$$(5.1) L_k w = v in \Omega,$$

$$(5.2) w = 0 on \partial \Omega,$$

exactly. Instead, we shall define an approximate solution $W = E_{kh}v$ in S_h^{μ} and take $u_{kh}(x, t) = E_{kh}^n v(x)$ for our solution at t = nk of the discrete problem. For the construction of the operator E_{kh} , we introduce the quadratic functional

$$\Lambda(\varphi;v) = ||L_k \varphi - v||^2 + \gamma_{kh} |\varphi|^2,$$

where γ_{kh} is a real number satisfying

$$\gamma k^{1/2} \le \gamma_{kh} \le C k^2 h^{-3},$$

where γ is the constant in Lemma 4.3. Notice that, by (5.3), we assume that kh^{-2} is bounded away from zero. Further, we introduce, for φ , $\psi \in H^2$,

$$((\varphi, \psi))_{\Lambda} = ((L_k \varphi, L_k \psi)) + \gamma_{kh}(\varphi, \psi),$$

$$||\varphi||_{\Lambda} = (||L_k \varphi||^2 + \gamma_{kh} |\varphi|^2)^{1/2}.$$

By the fact that (5.1), (5.2) with v = 0 only admits the trivial solution w = 0, this defines an inner product and a norm on H^2 .

According to the following lemma, we can now define $W = E_{kh}v$ as the function which minimizes $\Lambda(\varphi; v)$ as φ varies through S_h^{μ} .

LEMMA 5.1. There is a unique $W \in S_h^{\mu}$ minimizing $\Lambda(\varphi; v)$. This is the unique solution in S_h^{μ} of

$$((W, f))_{\Lambda} = ((v, L_k f))$$
 for all $f \in S_h^{\mu}$.

Proof. Recalling that $w = E_k v$ denotes the exact solution of (5.1), (5.2), we can write

$$\Lambda(\varphi;v) = ||\varphi - E_k v||_{\Lambda}^2$$

and, hence, Λ is minimized by the unique $W \in S^{\mu}_{h}$ which satisfies

$$((W - w, f))_{\Lambda} = 0$$
 for all $f \in S_h^{\mu}$.

Since, by (5.1), (5.2), $((w, f))_{\Lambda} = ((v, L_k f))$, the lemma is proved.

The operator E_{kh} defined above is bounded in L_2 .

LEMMA 5.2. We have, for $v \in L_2$,

$$||E_{kh}v|| \leq ||E_{kh}v||_{\Lambda} \leq ||v||.$$

Proof. By Lemma 5.1, we have, with $W = E_{kh}v$,

$$||W||_{\Lambda}^{2} \leq ||v|| \cdot ||L_{k}W|| \leq ||v|| ||W||_{\Lambda}.$$

Since on the other hand by Lemma 4.3, $||W|| \le ||W||_{\Lambda}$, the result follows.

LEMMA 5.3. Let $0 \le s \le \mu$. Then there is a constant C such that, for $w \in \dot{H}^{2+s}$,

$$\inf_{\varphi \in S_h^{\mu}} ||\varphi - w||_{\Lambda} \leq Ckh^s ||w||_{2+s}.$$

Proof. We have, under the assumption (5.3) on γ_{kh} ,

$$||\varphi||_{\Lambda} \leq C(||\varphi|| + k||\varphi||_{H^{2}} + \gamma_{kh}^{1/2}|\varphi|)$$

$$\leq Ck(||\varphi||_{H^{2}} + h^{-2}||\varphi|| + h^{-3/2}|\varphi|)$$

and, hence, using Lemma 4.1 with $\epsilon = h^{1/2}$

$$||\varphi||_{\Lambda} \leq Ckh^{-2} \sum_{l=0}^{2} h^{l}||\varphi||_{H^{l}}.$$

Consequently, by the definition of S_h^{μ} ,

$$\inf_{\varphi \in S_h^{\mu}} ||\varphi - w||_{\Lambda} \leq Ckh^{-2} \inf_{\varphi \in S_h^{\mu}} \sum_{l=0}^{2} h^{l} ||\varphi - w||_{H^{l}} \leq Ckh^{s} ||w||_{2+s},$$

which proves the lemma.

LEMMA 5.4. We have, for $v \in \dot{H}^{\max(\mu+2,4)}$.

$$||E_{kh}v - E(k)v|| \leq C(kh^{\mu}||v||_{\mu+2} + k^{2}||v||_{4}),$$

and if $s \geq 0$, for $v \in \dot{H}^s$,

$$(5.5) ||E_{kh}v - E(k)v|| \leq ||E_{kh}v - E(k)v||_{\Lambda} \leq C(h^{\min(s,\mu)} + k^{\min(s/2,2)}) ||v||_{s}.$$

Proof. By Lemma 4.3, we have, using the definition of E_{kh} ,

$$||E_{kh}v - E_kv|| \leq ||E_{kh}v - E_kv||_{\Lambda} = \inf_{\varphi \in S_{h^{\mu}}} ||\varphi - E_kv||_{\Lambda},$$

and by Lemma 5.3 and Theorem 3.1,

$$(5.6) ||E_{kh}v - E_kv||_{\Lambda} \leq Ckh^{\mu}||E_kv||_{\mu+2} \leq Ckh^{\mu}||v||_{\mu+2}.$$

Together with Theorem 3.2, this proves (5.4). In addition to (5.6), we have, by Lemma 5.2,

$$||E_{kh}v - E_kv||_{\Lambda} \leq 2||v||,$$

and, hence, by interpolation (Lemma 2.2) for $0 \le s \le \mu + 2$,

$$||(E_{kh} - E_k)v||_{\Lambda} \le C(kh^{\mu})^{s/(\mu+2)}||v||_s \le C(h^s + k^{s/2})||v||_s.$$

Using once again Lemma 3.2, this implies (5.5) for $0 \le s \le \mu + 2$ and, hence, if $\mu \ge 2$, for all $s \ge 0$. For $\mu = 1$ and $s \ge 3$, we have obviously

$$||E_{kh}v - E_kv|| \le Ckh||v||_s \le Ch^{\min(s,1)}||v||_s$$

so that (5.5) holds also in this case.

THEOREM 5.1. Let E_{kh} satisfy the above assumptions. Then, for $s \ge 0$, T > 0, there is a constant C such that, for $v \in \dot{H}^s$ and $0 \le t = nk \le T$,

$$||E_{kh}(t)v - E(t)v|| \leq C \left\{ \left(\log \frac{T}{k} \right)^{\delta_{s,\mu}} h^{\min(s,\mu)} + \left(\log \frac{T}{k} \right)^{\delta_{s,s}} k^{\min(s/2,1)} \right\} ||v||_{s}.$$

Proof. We shall use the identity

$$E_{kh}(t)v - E(t)v = E_{kh}^n v - E(k)^n v = \sum_{i=0}^{n-1} E_{kh}^{n-1-i} (E_{kh} - E(k))E(jk)v,$$

and notice that, hence, by Lemma 5.2,

(5.7)
$$||E_{kh}(t)v - E(t)v|| \leq \sum_{i=0}^{n-1} ||(E_{kh} - E(k))E(jk)v||.$$

For j > 0, we have, by (5.4) and Theorem 2.1 for $s \le \min(\mu + 2, 4)$,

$$||(E_{kh} - E(k))E(jk)v|| \le Ckh^{\mu}||E(jk)v||_{\mu+2} + Ck^{2}||E(jk)v||_{4}$$

$$\le C\{kh^{\mu}(jk)^{-(\mu+2-s)/2} + k^{2}(jk)^{-(4-s)/2}\} ||v||_{s},$$

and, hence, by Lemma 4.5,

(5.8)
$$\sum_{i=1}^{n-1} ||(E_{kh} - E(k))E(jk)v|| \\ \leq C \left\{ h^{\mu} \left(\log \frac{T}{k} \right)^{\delta_{s,\mu}} k^{\min(0,(s-\mu)/2)} + k \left(\log \frac{T}{k} \right)^{\delta_{s,z}} k^{\min(0,(s-2)/2)} \right\} ||v||_{s}.$$

Taking into account the fact that $k \ge ch^2$, the result now follows from (5.5), (5.7), and (5.8). The case $s > \min(\mu + 2, 4)$ is treated similarly. This completes the proof of the theorem.

(b) The Crank-Nicolson Method. In order to define the approximate solution $W = \tilde{E}_{kh}v$ in S_h^{μ} of the Dirichlet problem

$$L_k^- w = L_k^+ v \quad \text{in } \Omega,$$

 $w = 0 \quad \text{on } \partial \Omega.$

we shall this time set

$$\tilde{\Lambda}(\varphi;v) = \left| \left| L_k^- \varphi - L_k^+ v \right| \right|^2 + \tilde{\gamma}_{kh} |\varphi|^2,$$

where $\tilde{\gamma}_{kh}$ satisfies $\gamma_{\alpha} \leq \tilde{\gamma}_{kh} \leq Ck^2h^{-3}$, where γ_{α} is the constant in Lemma 4.4. We also introduce the inner product and norm defined by

$$((\varphi, \psi))_{\tilde{\Lambda}} = ((L_k^- \varphi, L_k^- \psi)) + \tilde{\gamma}_{kh}(\varphi, \psi),$$

$$||\varphi||_{\tilde{\Lambda}} = (||L_k^- \varphi||^2 + \tilde{\gamma}_{kh}|\varphi|^2)^{1/2}.$$

In analogy with Lemma 5.1, we then have

LEMMA 5.5. There is a unique $W \in S_h^{\mu}$ minimizing $\tilde{\Lambda}(\varphi; v)$. This is the unique solution in S_h^{μ} of

$$((W, f))_{\tilde{\Lambda}} = ((L_k^+ v, L_k^- f))$$
 for all $f \in S_h^\mu$.

Proof. As above, we may write

$$\tilde{\Lambda}(\varphi;v) = ||\varphi - \tilde{E}_k v||_{\tilde{\Lambda}}^2,$$

so that the functional is minimized by W satisfying, for all $f \in S_h^\mu$,

$$((W, f))_{\tilde{\Lambda}} = ((\tilde{E}_k v, f))_{\tilde{\Lambda}} \equiv ((L_k^+ v, L_k^- f)).$$

If we set $\tilde{E}_{kh}v = W$ where W is defined in Lemma 5.5, our discrete solution at t = nk of the discrete problem is $\tilde{u}_{kh}(x, t) = \tilde{E}_{kh}^n v$.

LEMMA 5.6. The operator \tilde{E}_{kh} thus defined satisfies, for small k,

$$(5.9) ||\tilde{\mathcal{E}}_{kh}v|| \leq ||\tilde{\mathcal{E}}_{kh}v||_{\tilde{\Lambda}} \leq (1+\alpha k) ||v||_{\tilde{\Lambda}}$$

and, for $nk \leq T$,

$$(5.10) ||E_{hh}^n v|| \leq e^{\alpha T} ||v||_{\tilde{\Lambda}}.$$

Proof. Noticing that $L_k^- = L_{k/2}$ and that $\tilde{\gamma}_{kh} \ge \gamma k^{1/2}$ for small k, the first half of (5.9) follows by Lemma 4.3. By Lemma 5.5, we have, with f = W,

$$||W||_{\tilde{\Lambda}}^2 \leq ||L_k^+v|| ||W||_{\tilde{\Lambda}}.$$

On the other hand, by Lemma 4.4,

$$||L_k^+v|| \leq (1+\alpha k) ||v||_{\tilde{\Lambda}}.$$

Together, these last two inequalities prove the second half of (5.9). This immediately implies (5.10).

LEMMA 5.7. Let $0 \le s_1 \le \mu$, $0 \le s_2 \le 6$. Then, for $v \in \dot{H}^{\max(2+s_1,s_2)}$,

$$||\tilde{E}_{kh}v - E(k)v||_{\tilde{\Lambda}} \leq C(kh^{s_1}||v||_{2+s_1} + k^{s_2/2}||v||_{s_2}).$$

In particular, for any $s \ge 2$, and $v \in \dot{H}^s$,

$$(5.11) ||\tilde{\mathcal{E}}_{kh}v - E(k)v||_{\tilde{\Lambda}} \leq C(h^{\min(s,\mu)} + k^{\min(s/2,2)})||v||_{s}.$$

Proof. As in Lemma 5.3, we have

$$\inf_{\varphi \in S_h^{\mu}} ||\varphi - w||_{\tilde{\Lambda}} \leq Ckh^{s_1}||w||_{2+s_1},$$

and hence, using also Theorem 3.3,

$$(5.12) ||\tilde{E}_{kh}v - \tilde{E}_{k}v||_{\tilde{\Lambda}} \leq Ckh^{s_1}||\tilde{E}_{k}v||_{2+s_1} \leq Ckh^{s_1}||v||_{2+s_1}.$$

The first inequality then follows by Lemma 3.4. We now notice that, from (5.12), it follows by the inequality between the geometric and arithmetic means that, for $2 \le s \le 2 + \mu$,

$$||\tilde{E}_{kh}v - \tilde{E}_{k}v||_{\tilde{\Lambda}} \leq C(h^s + k^{s/2})||v||_{s},$$

which proves (5.11) for $2 \le s \le \mu + 2$. For $s > \mu + 2$, we have

$$||\tilde{E}_{kh}v - \tilde{E}_{k}v||_{\tilde{\Lambda}} \leq Ckh^{\mu}||v||_{2+\mu} \leq Ch^{\min(\mu,s)}||v||_{s}.$$

This completes the proof of the lemma.

THEOREM 5.2. For $s \ge 2$, T > 0, there is a constant C such that, for $v \in \dot{H}^s$ and $0 \le t = nk \le T$,

$$||\tilde{E}_{kh}(t)v - E(t)v|| \leq C \left\{ \left(\log \frac{T}{k} \right)^{\delta_{s,\mu}} h^{\min(s,\mu)} + \left(\log \frac{T}{k} \right)^{\delta_{s,\star}} k^{\min(s/2,2)} \right\} ||v||_{s}.$$

Proof. We have as in the proof of Theorem 5.1, using Lemma 5.6,

$$||\tilde{E}_{kh}(t)v - E(t)v|| \leq \sum_{j=0}^{n-1} ||\tilde{E}_{kh}^{n-1-j}(\tilde{E}_{kh} - E(k))E(jk)v||$$

$$\leq C \sum_{j=0}^{n-1} ||(\tilde{E}_{kh} - E(k))E(jk)v||_{\tilde{\Lambda}}.$$

By Lemma 5.7 and Theorem 2.1, we have, for $s \leq \min(\mu + 2, 6)$,

$$||(\tilde{E}_{kh} - E(k))E(jk)v||_{\tilde{\Lambda}} \leq C\{kh^{\mu}(jk)^{-(\mu+2-s)/2} + k^{3}(jk)^{-(\theta-s)/2}\}||v||_{s}$$

so that by Lemma 4.5,

$$(5.13) \qquad \sum_{j=1}^{n-1} ||(\tilde{E}_{kh} - E(k))E(jk)v||_{\tilde{\Lambda}} \\ \leq C \left\{ \left(\log \frac{T}{k} \right)^{\delta_{s,\mu}} h^{\min(s,\mu)} + \left(\log \frac{T}{k} \right)^{\delta_{s,\mu}} k^{\min(s/2,2)} \right\} ||v||_{s}.$$

The case $s > \min(\mu + 2, 6)$ is treated similarly. Together, (5.11) and (5.13) complete the proof.

(c) Some Modifications of the Crank-Nicolson Method. We shall consider briefly the situation $0 \le s < 2$. In this case, the method above demands more regularity than the initial-values possess. It is then natural to approximate the initial-values by smoother functions. More precisely, we shall consider an approximating operator P_h with the following property: For given s with $0 \le s \le 2$ there is a constant C such that if $v \in \dot{H}^s$, then $P_h v \in \dot{H}^2$ and

$$||P_h v||_2 \le Ch^{-(2-s)}||v||_s, \qquad ||P_h v - v|| \le Ch^s ||v||_s.$$

Such operators exist, as can easily be seen using the expansion (2.3) and the definition of $||\cdot||_s$. We then set $\tilde{E}'_{kh}(t) = \tilde{E}_{kh}(t)P_h$. For simplicity, we restrict ourselves to the case $\mu \ge 3$, that is, to the case when the accuracy in S^{μ}_h matches that of the discretization in time. We have

THEOREM 5.3. Let $\mu \ge 3$. For $0 \le s \le 2$, T > 0 there is a constant C such that, for $v \in \dot{H}^s$ and $0 \le t = nk \le T$,

$$||\tilde{E}'_{kh}(t)v - E(t)v|| \leq Ckh^{-(2-s)}||v||_{s}.$$

Proof. We have, using Theorem 5.2 and the definition of P_h ,

$$\begin{aligned} ||\tilde{E}'_{kh}(t)v - E(t)v|| &\leq ||(\tilde{E}_{kh}(t) - E(t))P_hv|| + ||E(t)(P_h - I)v|| \\ &\leq C(h^2 + k)||P_hv||_2 + C||P_hv - v|| \\ &\leq C((h^2 + k)h^{-(2-s)} + h^s)||v||_s \leq Ckh^{-(2-s)}||v||_s. \end{aligned}$$

The above method has an error estimate which for small s is unsatisfactory, since $kh^{-2} \ge ch^{-1/2}$. We shall, therefore, describe a method which does not have this deficiency. The modification consists in making the first step somewhat differently. Thus, with the above notation let $t = (n + \frac{1}{2})k$ and set $\tilde{E}'_{kh}(t) = \tilde{E}^n_{kh}E_{k/2.h}$. This amounts to taking the first half-step by the purely implicit method and using the result as initial-values for calculations with the Crank-Nicolson method. Notice that the assumption on $\tilde{\gamma}_{kh}$ is more restrictive than that on γ_{kh} .

We have the following:

THEOREM 5.4. For $s \ge 0$, T > 0, there is a constant C such that, for $v \in \dot{H}^s$ and $0 < t = (n + \frac{1}{2})k \le T$,

$$||\tilde{E}_{kh}^{\prime\prime}(t)v - E(t)v|| \leq C \left\{ \left(\log \frac{T}{k}\right)^{\delta_{s,\mu}} h^{\min(s,\mu)} + \left(\log \frac{T}{k}\right)^{\delta_{s,\star}} k^{\min(s/2,2)} \right\} ||v||_{s}.$$

Proof. We have

$$||\tilde{E}_{kh}^{"}(t)v - E(t)v|| \leq ||(\tilde{E}_{kh}^{n} - E(nk))E(\frac{1}{2}k)v|| + ||\tilde{E}_{kh}^{n}(E(\frac{1}{2}k) - E_{k/2,h})v||$$

$$= S_{1} + S_{2}.$$

For the first term, we have, as in the proof of Theorem 5.2,

$$S_{1} \leq \sum_{j=0}^{n-1} || \tilde{E}_{kh}^{m-1-j} (\tilde{E}_{kh} - E(k)) E((j+\frac{1}{2})k)v ||$$

$$\leq C \sum_{j=0}^{n-1} || (\tilde{E}_{kh} - E(k)) E((j+\frac{1}{2})k)v ||_{\tilde{\Lambda}}.$$

By Lemma 5.7 and Theorem 2.1, we have, for $s \leq \min(\mu + 2, 6)$,

$$||(\tilde{E}_{kh}-E(k))E((j+\frac{1}{2})k)v||_{\tilde{\Lambda}}$$

$$\leq C\{kh^{\mu}((j+\frac{1}{2})k)^{-(\mu+2-s)/2}+k^{3}((j+\frac{1}{2})k)^{-(6-s)/2}\}||v||_{s},$$

so that again, by Lemma 4.5,

$$S_1 \leq C \left\{ \left(\log \frac{T}{k} \right)^{\delta_{s,\mu}} h^{\min(s,\mu)} + \left(\log \frac{T}{k} \right)^{\delta_{s,\mu}} k^{\min(s/2,2)} \right\} ||v||_s,$$

and, similarly, for $s > \min(\mu + 2, 6)$. By Lemmas 5.6 and 3.2, we have

$$S_2 \leq C||(E_{k/2,h} - E(\frac{1}{2}k))v||_{\tilde{\Lambda}} \leq Ck^{\min(s/2,2)}||v||_s.$$

This completes the proof.

Department of Mathematics Cornell University Ithaca, New York 14850 Department of Mathematics Chalmers Institute of Technology and the University of Göteborg Göteborg, Sweden

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