

A CONVERGENT BOUNDARY INTEGRAL METHOD FOR THREE-DIMENSIONAL WATER WAVES

J. THOMAS BEALE

ABSTRACT. We design a boundary integral method for time-dependent, three-dimensional, doubly periodic water waves and prove that it converges with $O(h^3)$ accuracy, without restriction on amplitude. The moving surface is represented by grid points which are transported according to a computed velocity. An integral equation arising from potential theory is solved for the normal velocity. A new method is developed for the integration of singular integrals, in which the Green's function is regularized and an efficient local correction to the trapezoidal rule is computed. The sums replacing the singular integrals are treated as discrete versions of pseudodifferential operators and are shown to have mapping properties like the exact operators. The scheme is designed so that the error is governed by evolution equations which mimic the structure of the original problem, and in this way stability can be assured. The wave-like character of the exact equations of motion depends on the positivity of the operator which assigns to a function on the surface the normal derivative of its harmonic extension; similarly, the stability of the scheme depends on maintaining this property for the discrete operator. With n grid points, the scheme can be implemented with essentially $O(n)$ operations per time step.

1. INTRODUCTION

In this paper we design a semidiscrete numerical method of boundary integral type for computing time-dependent, doubly periodic, three-dimensional water waves. We prove that this method converges as long as the actual motion remains smooth, without restriction on its amplitude. While the full equations are difficult to work with analytically, boundary integral methods seem naturally suited to water wave motion. The surface is represented in Lagrangian coordinates, and grid points are moved according to a computed velocity. Because the flow is assumed irrotational, the motion is determined by quantities on the surface alone. However, the normal velocity must be found in terms of singular boundary integrals, using potential theory. The evolution has the character of nonlinear, nonlocal wave motion without dissipation. For this reason it seems that the stability of the numerical method depends critically on its design. In the present work we develop a new, efficient approach for calculating the singular integrals, using the limited information computed on the moving surface. We analyze discrete versions of integral operators such as single and double layer potentials by adapting the viewpoint

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of pseudodifferential operators, as well as potential theory, to the discrete setting. We find the most important terms in the evolution equations for the errors, and ensure by design of the scheme that the errors grow at a bounded rate.

Boundary integral methods have been widely used in ocean engineering and applied mathematics, starting with the work of Longuet-Higgins and Cokelet [21] and Vinje and Brevig [33]. Two-dimensional applications have been extensive; see the recent surveys [27, 32] or the references in [5, 6]. Computations in 3-D include [4, 27, 28, 9, 32, 17]. In [6], T. Hou, J. Lowengrub, and the author proved the convergence of a version of the method in 2-D. Calculations illustrate the advantage of this method in capturing small scale features. It seems that convergence in 3-D is more difficult, largely because quadrature for singular integrals on surfaces is more involved than on curves, and because the choice of quadrature affects the stability of the time-dependent solution. One approach is presented in [19].

We assume as usual that the flow of the water is incompressible, inviscid, and irrotational. For simplicity we assume the fluid is infinitely deep and the motion is periodic in both horizontal directions, with period 2π . (The formulation can easily be modified to account for a horizontal bottom; for more general lower boundaries, see [3].) The motion of the fluid is governed by Euler's equations and boundary conditions at the surface. Since the flow is irrotational and incompressible, the velocity is the gradient of a potential ϕ which is harmonic below the surface:

$$(1.1) \quad \Delta\phi = 0.$$

At the surface the fluid pressure matches the atmospheric pressure, which we assume constant. (We neglect surface tension.) Bernoulli's equation, together with the boundary condition for the pressure, provides us with an evolution equation for ϕ at the surface. With the position x and velocity potential ϕ at the surface treated as functions of Lagrangian coordinates $\alpha = (\alpha_1, \alpha_2)$ and time t , the evolution equations are

$$(1.2) \quad x_t = v, \quad \phi_t = \frac{1}{2}|v|^2 - gx_3,$$

where v is the fluid velocity, g is the acceleration of gravity, x_3 is the vertical component of x , and ϕ is adjusted by a spatial constant at each t . The first equation says that a particle on the surface with fixed α moves with the fluid velocity. The velocity $v = \nabla\phi$ is determined by ϕ on the surface and the condition (1.1), with the requirement that $\nabla\phi$ is square integrable as $x_3 \rightarrow -\infty$.

In the boundary integral approach, the main effort in solving these equations is in finding the velocity v at the surface using potential theory. There is some choice in how this is done. The tangential part of the velocity can be found from differentiating ϕ along the surface. For the normal component we use a Fredholm integral equation of the second kind which determines the normal velocity $\phi_n = \partial\phi/\partial n$ directly from ϕ on the surface,

$$(1.3) \quad \frac{1}{2}\phi_n(x) + \int \frac{\partial G^\pi(x-y)}{\partial n(x)} \phi_n(y) dS(y) \\ = n(x) \cdot \int \nabla G^\pi(x-y) \times ((n(y) \times \nabla^T \phi(y)) dS(y).$$

Here G^π is the Green's function, periodic in the horizontal variables, obtained from a sum of images of the standard Green's function $G(x) = -1/4\pi|x|$ with $\Delta G = \delta$; n is the unit normal pointing out of the fluid. We assume ϕ is periodic and has square

integrable gradient below the surface. The first integral is absolutely convergent, but the second is of principal type. The right side is the normal derivative of the double layer potential due to ϕ . This integral equation has been used in electromagnetics. It can be derived by writing ϕ below the surface in terms of boundary integrals in ϕ and ϕ_n , and then taking the normal derivative at the surface (e.g., see [10], §3.9 and Theorem 2.23, or [20]). Its use for three-dimensional water waves has been suggested in [28]. An alternative approach is to write the velocity potential in terms of a dipole source on the boundary; this was done in [3, 4, 17, 5, 6].

To design a specific scheme, we have choices to make in writing the integrals, finding derivatives, and especially in the numerical integration of the singular integrals. Analytical considerations in the present work and in [6] indicate that these choices can determine whether or not the scheme is stable. There are well developed methods for quadrature of singular integrals in several dimensions which depend on special coordinates near the singularity; see Lyness [24] for a survey. In the present context the surface and integrand are known only from computed values at the Lagrangian grid points. Here we develop a general approach in which we replace the Green's function G by a smooth version G_h regularized on the scale of the grid size h . We discretize the new integral by the trapezoidal rule. Then, using an asymptotic expansion of the quadrature error like that found by Lyness [23] and Goodman et al. [12] for unregularized singular integrals, we identify the largest error term. Because of the regularization, we can compute this first error and correct for it; it is expressed through the Poisson summation formula in terms of the Fourier transform \hat{G}_h of G_h . In our case the correction improves an $O(h)$ error to $O(h^3)$. (We have avoided using extrapolation as in [23] for the sake of a positivity requirement explained below.)

As in [6] we are guided in designing the scheme by the linearization of the exact equations about an arbitrary solution. By preserving the same structure at the discrete level we can ensure that the numerical scheme is stable. Without such considerations we could have a mismatch of terms which destroys the well-posedness of the linearization and therefore the numerical stability. Briefly, this linearization reduces to an equation for a variable u related to the disturbance in the velocity potential on the surface,

$$(1.4) \quad u_{tt} + c\Lambda u \approx 0,$$

where we have dropped less important terms, and Λ is the principal part of the Dirichlet-to-Neumann operator on the current surface, i.e., the operator that determines ϕ_n from ϕ . It is important that Λ and c are positive, as discussed further below. The equation describes nonlocal wave motion; in the special case of small disturbances at equilibrium, it reduces to the usual equation for linearized water waves. The linearization about an arbitrary motion was found in the boundary integral setting in 2-D in [5], and in 3-D with orthogonal coordinates in [18]. It was derived earlier for bounded domains in a different way in [2].

A primary concern is that the discrete version of the operator Λ should be positive, or almost so. Violation of this requirement in high wavenumbers would lead to rapid growth of disturbances, as can be seen from (1.4). For the exact operator Λ , the positivity is related to the fact that the Green's function has transform $\hat{G} < 0$. This property may not be preserved by the discrete analogue. In the present approach, we choose G_h so that $\hat{G}_h < 0$. The discrete transform is a lattice sum of

values of \hat{G}_h , which converges because G_h is regularized. In this way we can ensure the necessary positivity.

We now describe the method in more detail. We first rewrite the integrals in (1.3) to reduce the order of singularity, taking advantage of the two identities

$$(1.5) \quad \int \frac{\partial G^\pi(x-y)}{\partial n(y)} dS(y) = 0, \quad \int \nabla G^\pi(x-y) \times n(y) dS(y) = 0,$$

where the integral is over one period of the surface. (Cf. [4], §3 or [10], Theorem 2.1. The use of these identities to reduce the singularity was suggested in [4].) On the right side of (1.3) we use vector identities to convert the integrand,

$$(1.6) \quad \begin{aligned} \nabla G^\pi \times (n \times \nabla^T \phi) &= (\nabla G^\pi \cdot \nabla^T \phi) n - (\nabla G^\pi \cdot n) \nabla^T \phi \\ &= (\nabla G^\pi \times n) \times \nabla^T \phi - (\nabla G^\pi \cdot n) \nabla^T \phi. \end{aligned}$$

Then using (1.5) we can write the integral on the right in (1.3) as

$$(1.7) \quad \begin{aligned} \int (\nabla G^\pi \times n(y)) \times (\nabla^T \phi(y) - \nabla^T \phi(x)) dS(y) \\ - \int \nabla G^\pi \cdot n(y) (\nabla^T \phi(y) - \nabla^T \phi(x)) dS(y). \end{aligned}$$

The first integral is absolutely convergent because of the subtraction. We can replace ∇G^π by $\nabla^T G^\pi$, the part of the gradient tangential at y , and write (cf. [10], p. 35), with $y = y(\alpha')$ and X_1, X_2 the tangent vectors $X_j = \partial y / \partial \alpha'_j$,

$$(1.8) \quad \nabla G^\pi(x-y) \times N(y) = (D_{\alpha'_1} G^\pi) X_2 - (D_{\alpha'_2} G^\pi) X_1.$$

Here $N = X_1 \times X_2$; we assume N points outward, so that $n = N/|N|$. For the integral on the left in (1.3), we resolve ∇G^π into parts normal and tangential at y and use (1.5) again, so that the integral becomes

$$(1.9) \quad \int \nabla G^\pi \cdot n(y) [n(y) \cdot n(x) \phi_n(y) - \phi_n(x)] dS(y) + \int \nabla^T G^\pi \cdot n(x) \phi_n(y) dS(y).$$

The second integrand is absolutely integrable, since $\nabla^T G^\pi \perp n(x)$ at $y = x$.

We work with grid functions on a grid of size h representing equally spaced values of the Lagrangian variable, $\alpha_j = jh$, where $j = (j_1, j_2) \in \mathbf{Z}^2$. We assume $h = 2\pi/N$ with N even. For the discrete values in a fundamental period we take

$$(1.10) \quad I = \{j \in \mathbf{Z}^2 : -N/2 \leq j_\nu \leq N/2 - 1, \nu = 1, 2\}.$$

A grid function f has a discrete Fourier transform which we denote by \check{f} , a function of $k \in \mathbf{Z}^2$ with period $2\pi/h$ in k_1, k_2 ,

$$(1.11) \quad \check{f}(k) = (2\pi)^{-2} \sum_{j \in I} f(jh) e^{-ikjh} h^2, \quad f(jh) = \sum_{k \in I} \check{f}(k) e^{ikjh}.$$

For properties of this transform see e.g., [15, 31]. We measure grid functions on Ih in the discrete L_h^2 norm, given by

$$(1.12) \quad |f|_{L_h^2}^2 = \sum_{j \in I} |f(jh)|^2 h^2 = (2\pi)^2 \sum_{k \in I} |\check{f}(k)|^2.$$

Of the exact solution, we assume that the surface function $x(\alpha, t)$ and the velocity potential $\phi(\alpha, t)$ are smooth up to some time T , and $x(\alpha_1, \alpha_2, t) - (\alpha_1, \alpha_2, 0)$ and $\phi(\alpha_1, \alpha_2, t)$ are 2π -periodic in each of α_1, α_2 . (If the velocity is periodic but ϕ is

not, we can choose a frame of reference so that ϕ becomes periodic. The scheme can easily be adapted to the more general case.) We also assume that the Jacobian $\partial x/\partial\alpha$ is nondegenerate and $x(\alpha, t) \neq x(\alpha', t)$ when $\alpha \neq \alpha'$. This implies that

$$(1.13) \quad |x(\alpha, t) - x(\alpha', t)| \geq c|\alpha - \alpha'|, \quad 0 \leq t \leq T.$$

Next we discuss the discrete derivative operator. It can be a difference operator, but to be general we discuss its Fourier representation. For a function f of $\alpha_j \in Ih$, we assume the discrete partial derivative $D_{h,\nu}$ in $\alpha_\nu, \nu = 1, 2$, has the form

$$(1.14) \quad (D_{h,\nu}f)^\cdot(k) = h^{-1}\sigma(k_\nu h)\check{f}(k), \quad \sigma(\xi + 2\pi) = \sigma(\xi),$$

where $\sigma : \mathbf{R} \rightarrow \mathbf{C}$. We also assume

$$(1.15) \quad \sigma \text{ is } C^1 \text{ on } [-\pi, \pi], \quad \sigma(-\pi) = \sigma(\pi), \quad C_1|\xi| \leq |\sigma(\xi)| \leq C_2|\xi| \text{ on } [-\pi, \pi],$$

$$(1.16) \quad \sigma(\xi) = i\xi + O(\xi^4) \text{ as } \xi \rightarrow 0, \quad \sigma(-\xi) = \bar{\sigma}(\xi),$$

where $\bar{\sigma}$ is the complex conjugate. The latter says that $D_{h,\nu}$ is accurate to $O(h^3)$ and preserves real-valued functions. Because of (1.15), $D_{h,\nu}$ has a product rule: for $f \in L_h^2$ and u a smooth periodic function,

$$(1.17) \quad D_{h,\nu}(uf) = uD_{h,\nu}f + B(f),$$

where B is an operator depending on u , bounded on L_h^2 uniformly in h (see [6], Lemma 1). This will be useful later. The requirement $\sigma(\xi) \neq 0$ for $\xi \neq 0$ rules out, e.g., the symmetric fourth order difference operator. A simple example meeting these conditions is the third order difference operator coming from Lagrange interpolation,

$$(1.18) \quad D_{h,\nu} = (6h)^{-1} (-2S_\nu^{-1} - 3I + 6S_\nu - S_\nu^2),$$

where S_ν is the shift operator, $S_1 f(j_1 h, j_2 h) = f((j_1 + 1)h, j_2 h)$. Alternatively, we could define σ directly, e.g., by setting $\sigma = i\xi\rho + (1 - \rho)$ for $|\xi| \leq \pi$, where $\rho(\xi)$ is some even, real-valued function with $\rho \equiv 1$ near $\xi = 0$ and $\rho \equiv 0$ near $\xi = \pm\pi$. We shall refer to the adjoint operator $D_{h,\nu}^*$, given by

$$(1.19) \quad (D_{h,\nu}^*f)^\cdot(k) = h^{-1}\bar{\sigma}(k_\nu h)\check{f}(k).$$

Of course, for (1.18), $D_{h,\nu}^*$ is found by replacing S_ν with S_ν^{-1} . For f smooth, $D_{h,\nu}f = \partial f/\partial\alpha_\nu + O(h^3)$ while $D_{h,\nu}^*f = -\partial f/\partial\alpha_\nu + O(h^3)$.

Various geometric quantities must be computed from the grid points on the surface. From $x(\alpha_j), j \in I$, we can use $D_{h,\nu}$ to compute approximate tangent vectors $X_{\nu j} = (D_{h,\nu}x)_j, \nu = 1, 2$. (We apply $D_{h,\nu}$ to $x(\alpha) - (\alpha, 0)$.) From these we compute the metric tensor $g_{\mu\nu} = X_\mu \cdot X_\nu$ and the inverse $g^{\mu\nu}$, as functions of α_j . We then find the normal vectors $N = X_1 \times X_2$ and $n = N/|N|$, and also the dual tangent vectors at α_j ,

$$(1.20) \quad X_\mu^* = \sum_\nu g^{\mu\nu} X_\nu, \quad X_\mu^* \cdot X_\nu = \delta_{\mu\nu}.$$

Given the surface x and the velocity potential ϕ at the surface at one time for the grid points $\alpha_j, j \in I$, we can advance to the next time using (1.2) once we have computed the velocity v at each α_j . To do this we write the computed velocity as

$$(1.21) \quad v = \nabla_h^T \phi + wn,$$

where w is an approximation to ϕ_n . We can compute the tangential gradient as (e.g., cf. [10], p. 33)

$$(1.22) \quad \nabla_h^T \phi = \sum_{\nu=1,2} (D_{h,\nu} \phi) X_\nu^*.$$

We will obtain w from a discrete version of (1.3), rewriting the two integrals as in (1.7)–(1.9). We use the regularized Green’s function G_h^π ; for the normal derivatives we use the analytic gradient of G_h^π , while for $\nabla^T G_h^\pi(x - x(\alpha'))$, the part of the gradient tangential at $x(\alpha')$, we use the discrete α' -derivative,

$$(1.23) \quad \nabla_h^T G_h^\pi(x - x(\alpha')) = - \sum_{\nu=1,2} (D_{h,\nu} G_h^\pi(x - x(\alpha'))) X_\nu^*.$$

This expression is used to match (1.22); both appear in the discrete operator Λ mentioned above, and this symmetry gives it the proper structure.

The regularized Green’s function G_h^π is constructed in §2 from a free space version in the form $G_h(x) = -(4\pi|x|)^{-1} s(|x|/h)$ for $x \in R^3$, where s is a function chosen with certain conditions (2.2), (2.3), (2.9) which ensure that G_h is smooth and differs from G itself as an integral operator by $O(h^3)$. As above, we also assume that $\hat{G}_h(k) < 0$. A specific choice (2.19) for s is described in §2, based on the Gaussian function, for which the requirements are satisfied and necessary quantities can be computed explicitly. Since the regularization has length scale h , G_h differs appreciably from G only within distance $O(h)$ of the origin. If, for example, $x(\alpha) = (\alpha_1, \alpha_2, 0)$ and we approximate the single layer potential due to a function f by applying the trapezoidal rule with G_h in place of G , we have (with a limiting value at $\ell = j$)

$$(1.24) \quad \sum_{\ell \in \mathbf{Z}^2} G((jh - \ell h, 0)) s(j - \ell) f(\ell h) h^2,$$

and the s factor amounts to a set of quadrature weights. The quadrature error is $O(h)$; however, it can be improved to $O(h^3)$ by a correction proportional to $f(jh)$, as explained in §3. Such corrections appear in the discrete integrals below.

The discrete integral equation is obtained by substituting (1.7), (1.9) into (1.3) for the two integrals, replacing G^π with G_h^π , applying the trapezoidal rule, and adding the needed quadrature correction. It has the form

$$(1.25) \quad \frac{1}{2} w_j + (\mathcal{K}_h w)_j = f_j = F_j \cdot n_j,$$

$$(1.26)$$

$$(\mathcal{K}_h w)_j = \sum_{\ell} \nabla G_h^\pi \cdot N_\ell [(n_\ell \cdot n_j) w_\ell - w_j] h^2 + \sum_{\ell} \nabla_h^T G_h^\pi \cdot n_j w_\ell |N_\ell| h^2 + h \kappa_j w_j$$

$$(1.27)$$

$$F_j = \sum_{\ell} [D_h G_h^\pi, X]_\ell \times (\nabla_h^T \phi_\ell - \nabla_h^T \phi_j) h^2 + h \chi_j - \sum_{\ell} \nabla G_h^\pi \cdot N_\ell (\nabla_h^T \phi_\ell - \nabla_h^T \phi_j) h^2$$

Here $\nabla_h^T \phi$ is found from (1.22) and $\nabla_h^T G_h^\pi$ from (1.23); ∇G_h^π etc. are evaluated at $x_j - x_\ell$; and in view of (1.8) we have introduced

$$(1.28) \quad [D_h G_h^\pi, X]_\ell = D_{h,1} G_h^\pi(x_j - x_\ell) X_{2\ell} - D_{h,2} G_h^\pi(x_j - x_\ell) X_{1\ell},$$

where D_h is with respect to ℓ . The correction terms are given by

$$(1.29) \quad \kappa_j = \gamma_j [P_h(D_{h,1}^* X_1^* + D_{h,2}^* X_2^*)]_j \cdot N_j,$$

$$(1.30) \quad \chi_j = \gamma_j (X_{1j} \times [P_h D_{h,2}^* (\nabla_h^T \phi)]_j - X_{2j} \times [P_h D_{h,1}^* (\nabla_h^T \phi)]_j),$$

where

$$(1.31) \quad \gamma_j = 2\pi (\det g^{\mu\nu}(\alpha_j))^{1/2} \sum_{0 \neq n \in \mathbf{Z}^2} \Gamma \left(2\pi \sqrt{g^{\mu\nu}(\alpha_j) n_\mu n_\nu} \right)$$

and Γ is a function related to G_h ; see (2.14), (2.24). The sum in (1.31) is infinite, but we can choose G_h so that Γ decreases rapidly and only a few terms are needed (cf. (2.24)). The derivation of these corrections is explained in §3. A linear operator P_h is inserted in (1.29), (1.30) to smooth out the second derivatives. We assume it has the form

$$(1.32) \quad (P_h f)^\sim(k) = \rho(k\sqrt{h}) \ddot{f}(k)$$

with ρ chosen so that

$$(1.33) \quad \rho(\xi) = 1 + O(|\xi|^4) \text{ as } \xi \rightarrow 0, \quad \rho(\xi) = 0 \text{ for } |\xi| > c_0, \quad c_0 > 0.$$

As part of the convergence argument, we prove that the integral equation can be solved by simple iteration, i.e.,

$$(1.34) \quad \frac{1}{2} w^{(n+1)} + \mathcal{K}_h w^{(n)} = f, \quad w^{(0)} = f.$$

The following theorem gives the convergence result for this scheme.

Main Theorem. *Suppose an initial state is prescribed, such that the exact equations of motion (1.1), (1.2) have a smooth solution for $0 \leq t \leq T$ meeting the conditions above (1.13). Let the numerical scheme be as presented, with the discrete derivative $D_{h,\nu}$ chosen according to (1.14)–(1.16) and the operator P_h as in (1.32), (1.33). Let G_h be a regularized Green’s function satisfying (2.1)–(2.3), (2.9) and $\hat{G}_h < 0$. Then for h sufficiently small, the scheme has a solution with the prescribed initial state for $0 \leq t \leq T$, and in particular the discrete integral equation (1.25) can be solved. For each time $t \leq T$, the surface computed at the grid points α_j differs from the exact surface by $O(h^3)$ in L_h^2 . The computed velocity potential at the surface has error $O(h^3)$ in L_h^2 , and the computed velocity at the surface has error $O(h^2)$ in L_h^2 .*

This scheme is semidiscrete, i.e., discrete in space but not time. We expect the time integration to be done using an ODE solver such as the Runge-Kutta or Adams-Bashforth methods. Higher order versions of this scheme are possible but would require more complicated correction terms. We do not deal in detail here with the efficient computation of the discrete integrals; it is important to note, however, that with $n = N^2$ points to be tracked, the computation can be done in essentially $O(n)$ operations per time step. The four integrals can be put in matrix-vector form, where the matrix comes from either G_h^π or its gradient. There are two ways to proceed, based on the fast multipole method of Greengard and Rokhlin [14] or Ewald summation. Both have been used for doubly periodic water wave computations [4, 17]. We can choose the regularization of the Green’s function, e.g., (2.19), so that it is significant only at distance $O(h)$ from the singularity. Then fast summation can be used except for $O(1)$ terms per integral, or $O(n)$ terms in total. An alternative is to adapt the fast version of Ewald summation of Strain [29].

As usual, the theorem asserts the convergence of the scheme as long as a smooth solution exists. Recently Sijue Wu has proved that a smooth solution of the initial value problem for water waves exists for a time depending on the initial state, in a three-dimensional fluid of infinite extent, tending to equilibrium at infinity [35]. (Earlier results were two-dimensional or assumed analytic data.) It is reasonable to expect that a result similar to Wu's holds for the present case of doubly periodic motion. Wu shows in her case that the pressure gradient at the surface is bounded away from zero,

$$(1.35) \quad c = -\nabla p \cdot n \geq c_0 > 0,$$

where n is the normal outward from the fluid region. Such a result was proved for a bounded domain in [2]. The same condition holds in the present case; this can be seen as in §4 of [35]. The essential reason is that $-p$ is subharmonic and therefore obeys the strict maximum principle. The coefficient (1.35) appears in (1.4). The positivity is important for the well-posedness of the exact equations and consequently also for the numerical stability of the scheme under consideration, as seen in §6. It means that the motion is well-posed even after a wave overturns. (Of course the model ceases to apply once the wave crashes.) Further discussion of the significance of (1.35) can be found in [5].

In analyzing the stability of the scheme we need to understand the mapping properties of the discrete integral operators applied to error terms. It is natural to view them as discrete versions of pseudodifferential operators; the important parts can be regarded as convolutions and estimated in the Fourier transform. This point of view is especially helpful in establishing the positivity of the operator Λ using the assumption $\hat{G}_h < 0$. In §4 we develop some basic properties of discrete pseudodifferential operators under mild conditions, including a version of Gårding's inequality. In [25] general results for such operators were derived assuming a high wavenumber cut-off. Here we avoid this assumption and derive more limited results. In §5 we show that various discrete operators related to G_h^π are bounded, or gain derivatives, as linear operators on L_h^2 . These are discrete versions of standard properties of single and double layer potentials. In the stability estimates of §6 we use these mapping properties to identify the principal error terms and simplify them, without treating less important terms in detail. The singularity subtraction helps to prevent spurious terms from appearing in the stability analysis. In fact, a scheme in 2-D like that of [6] can be shown to converge if singularity subtraction is used, without smoothing the points x_j inside the integrals, as was done in [6].

We briefly outline the contents of the remaining sections. In §2 we describe the regularized Green's function G_h and derive needed formulas, construct the periodic version G_h^π , and prove that the error from replacing G^π with G_h^π in a single or double layer potential is $O(h^3)$. In §3 we analyze the quadrature error for the trapezoidal rule applied to singular integrals with regularization, and derive a formula to remove the largest error by local correction. We apply these results to the discrete integrals of (1.26), (1.27). In §4 we prove basic properties of discrete pseudodifferential operators, and in §5 the boundedness properties of discrete integral operators. The convergence of the scheme is proved in §6: stability estimates are obtained for the computed velocity, using the results of §§4 and 5; a simplified equation is found for the growth of the error; and estimates are found for the rate of growth. Some arguments needed for the proof are deferred to §7.

The operator Λ is essentially a convolution with $\nabla^T G$, following a derivative; see Lemma 6.8 and (6.31) for the discrete version. The positivity of the discrete Λ depends on the choice of quadrature for the singular integral, as well as the choice of the two derivatives. It appears difficult to maintain this condition in discretizing the integral without regularizing G ; the sign condition on \hat{G}_h and the matching of the two derivatives ensure the positivity here. In the stability argument of §6, the positivity of Λ is needed because it enters the energy estimates; see (6.55). We also need the discrete Λ to dominate the discrete first derivative, i.e., the derivative can be written as a bounded operator times Λ (see (6.49)–(6.50)). It is for this latter reason that we require the derivative in (1.14) to have nonzero symbol σ for $k \neq 0$; if σ decays in the high wavenumbers, then the symbol of Λ decays faster, since Λ has two derivatives. In the 2-D convergence argument of [6], the analogue of $\nabla^T G$ was the Hilbert transform H ; the discrete H given by alternate quadrature had symbol with modulus one, and the two needed properties of $\Lambda = HD$ followed directly.

2. THE REGULARIZED GREEN’S FUNCTION

In this section we describe the class of regularized Green’s functions and find the Fourier transform of the restriction to a plane in terms of the 3-D transform. We need to compute this transform explicitly for the correction terms in the integral equation (1.25). We find a specific G_h , based on the Gaussian function, which has all the needed properties. We construct the periodic Green’s function as a sum of images, adjusted by constants. Finally, we prove (Theorems 2.2 and 2.3) that the error in a single or double layer potential due to the regularization is $O(h^3)$.

The regularized Green’s function G_h will have the form

$$(2.1) \quad G_h(x) = -(4\pi r)^{-1} s(r/h), \quad r = |x|,$$

with s chosen so that $s(r) \rightarrow 1$ rapidly as $r \rightarrow \infty$ and G_h is smooth. A convenient assumption for the decay of $s - 1$ is

$$(2.2) \quad |D_r^k (s(r) - 1)| \leq Cr^{-4-k}, \quad r \geq 1.$$

For G_h to be smooth, we need $s(|x|)/|x|$ to be smooth as a function of x , and thus as a function of $|x|^2$; i.e., we assume

$$(2.3) \quad s(r)/r \text{ is a smooth function of } r^2, \quad 0 \leq r < \infty.$$

Then for $h > 0$, $G_h(x) = h^{-1}G_1(x/h)$. For later use we note that (cf. [1])

$$(2.4) \quad |D_x^k G_h(x)| \leq \begin{cases} C|x|^{-|k|-1}, & |x| \geq h, \\ Ch^{-|k|-1}, & |x| \leq h. \end{cases}$$

Letting $\psi = \Delta G_1$, we find that

$$(2.5) \quad \psi(x) = \Delta G_1(x) = -(4\pi r)^{-1} s''(r), \quad r = |x|,$$

and correspondingly

$$(2.6) \quad \Delta G_h(x) = \psi_h(x) \equiv h^{-3} \psi(|x|/h),$$

which approximates the delta function as $h \rightarrow 0$.

For accuracy we need a further condition on s . It is well-known (e.g., [16]) that the error from replacing G by G_h in an integral is determined by moments of $s - 1$

or ψ . Here we are interested in integrals on a surface, and so we consider, for a homogeneous polynomial $p_n(x)$ of degree n , the integral

$$(2.7) \quad \int_{\mathbf{R}^2} (G_h(x) - G(x)) p_n(x) dx = -\frac{1}{4\pi} \int_{\mathbf{R}^2} (s(|x|/h) - 1) |x|^{-1} p_n(x) dx,$$

which becomes in polar coordinates

$$(2.8) \quad C_n \int_0^\infty (s(r/h) - 1) r^n dr = C_n h^{n+1} \int_0^\infty (s(\rho) - 1) \rho^n d\rho.$$

The largest error is $O(h)$ with $n = 0$. For this reason we require of s that

$$(2.9) \quad \int_0^\infty (s(r) - 1) dr = 0.$$

For odd n , the error terms above are zero since the integrand is odd. Thus with condition (2.9) we expect the error from the regularization to be $O(h^3)$. This is verified for single layer potentials in Theorem 2.2. Given an arbitrary $s_{(1)}$ satisfying (2.2), (2.3), we can easily produce a related function satisfying (2.9), as well as (2.2), (2.3), by setting

$$(2.10) \quad s_{(3)}(r) = s_{(1)}(r) + r \partial_r s_{(1)}(r).$$

Condition (2.9) can be verified for $s_{(3)}$ by an integration by parts. The corresponding relationship for the ψ 's is $\psi_{(3)} = 4\psi_{(1)} + r \partial_r \psi_{(1)}$. (A similar strategy for satisfying moment conditions was used in [8].)

When G_h has the form (2.1), we have a similar expression for ∇G_h ,

$$(2.11) \quad \nabla G_h(x) = \frac{x}{4\pi r^3} \tilde{s}(r/h), \quad \tilde{s}(r) = s(r) - r \partial_r s(r).$$

Here \tilde{s} has the same properties (2.2), (2.3) as s . If s satisfies the moment condition (2.9), then the same holds for \tilde{s} ; this can be seen by an integration by parts.

We need explicit formulas for \hat{G}_h , the Fourier transform of G_h in \mathbf{R}^3 , and for the transform of G_h on planes, since we work with integrals on surfaces. We will write the Fourier transform of a function f on \mathbf{R}^d as

$$(2.12) \quad \hat{f}(k) = (2\pi)^{-d/2} \int f(x) e^{-ikx} dx, \quad f(k) = (2\pi)^{-d/2} \int \hat{f}(k) e^{ikx} dk.$$

The hypotheses imply that $\hat{G}_h(k)$ is smooth for $k \neq 0$ and decays rapidly for large k . More particularly, it will be important to require that $\hat{G}_h(k) < 0$. Since $-|k|^2 \hat{G}(k) = \hat{\psi}(k)$, this is equivalent to requiring that $\hat{\psi}(k) > 0$. To find the transform of the restriction to a plane, we first identify $(x_1, x_2) \in \mathbf{R}^2$ with $(x_1, x_2, 0) \in \mathbf{R}^3$. Then the Fourier transform of the function on \mathbf{R}^2 given by $x \rightarrow G_h(x, 0)$ is

$$(2.13) \quad G_1(\cdot, 0)^\wedge(k_1, k_2) = (2\pi)^{-1/2} \int_{-\infty}^\infty \hat{G}_1(k_1, k_2, k_3) dk_3.$$

Since \hat{G}_1 is radial, this depends only on $|(k_1, k_2)|$, and we write $G_1(\cdot, 0)^\wedge(k_1, k_2) = \Gamma(|(k_1, k_2)|)$, with Γ defined by

$$(2.14) \quad \Gamma(\rho) = (2\pi)^{-1/2} \int_{-\infty}^\infty \hat{G}_1(\rho, 0, \ell) d\ell.$$

More generally we will use the transform of $G_1 \circ J : \mathbf{R}^2 \rightarrow \mathbf{R}$, given by $\alpha \rightarrow G_1(J\alpha)$, where $J : \mathbf{R}^2 \rightarrow \mathbf{R}^3$ is a 3×2 matrix. In our applications J will be the Jacobian

matrix of a coordinate mapping. Since G_1 is radial, $G_1(J\alpha)$ is a function of $|J\alpha|^2 = |J^*J\alpha \cdot \alpha|^2 = |B\alpha|^2$, where $B = (J^*J)^{1/2}$. Thus $G_1 \circ J(\alpha) = G_1(B\alpha, 0)$, and

$$(2.15) \quad (G_1 \circ J)^\wedge(k) = (\det B)^{-1} G_1(\cdot, 0)^\wedge(B^{-1}k), \quad k \in \mathbf{R}^2 - \{0\}.$$

We can now combine this with (2.13), using $|B^{-1}(k)| = |(J^*)^{-1}k|$, to obtain

$$(2.16) \quad (G_1 \circ J)^\wedge(k) = (\det J^*J)^{-1/2} \Gamma(|(J^*)^{-1}k|), \quad k \in \mathbf{R}^2 - \{0\}.$$

If the two columns of J are vectors $X_1, X_2 \in \mathbf{R}^3$, then $(J^*J)_{\mu\nu} = X_\mu \cdot X_\nu = g_{\mu\nu}$, the usual metric induced in the coordinate plane. Also $|(J^*)^{-1}k|^2 = g^{\mu\nu}k_\mu k_\nu$, summed over μ, ν , where $(g^{\mu\nu}) = (g_{\mu\nu})^{-1}$. Thus the formula above becomes

$$(2.17) \quad (G_1 \circ J)^\wedge(k) = (\det g_{\mu\nu})^{-1/2} \Gamma\left(\sqrt{g^{\mu\nu}k_\mu k_\nu}\right), \quad k \in \mathbf{R}^2 - \{0\}.$$

Of course $(G_1 \circ J)^\wedge(k) < 0$ since $\hat{G}_1 < 0$; this will be important later.

We now describe a specific choice of G_h which meets all our requirements. We start with the error function

$$(2.18) \quad \text{erf}(r) = \frac{2}{\sqrt{\pi}} \int_0^r e^{-s^2} ds.$$

It fulfills conditions (2.2), (2.3). Using (2.10), we define $s(r) = \text{erf}(r) + r \text{erf}'(r)$ or

$$(2.19) \quad s(r) = \text{erf}(r) + 2\pi^{-1/2} r e^{-r^2}$$

so that s satisfies the moment condition (2.9). For this s we find

$$(2.20) \quad \tilde{s}(r) = \text{erf}(r) + 2\pi^{-1/2}(2r^3 - r)e^{-r^2},$$

$$(2.21) \quad \psi(r) = \pi^{-3/2}(4 - 2r^2)e^{-r^2}.$$

As for the transform, we have

$$(2.22) \quad \hat{G}_1(k) = -(2\pi)^{-3/2} \left(\frac{1}{2} + |k|^{-2}\right) e^{-|k|^2/4}, \quad k \in \mathbf{R}^3.$$

Then, from the above,

$$(2.23) \quad \Gamma(\rho) = -(2\pi)^{-2} \int_{-\infty}^{\infty} \left(\frac{1}{2} + \frac{1}{\rho^2 + \ell^2}\right) e^{-(\rho^2 + \ell^2)/4} d\ell.$$

Using [13], formula 3.466, we have

$$(2.24) \quad \Gamma(\rho) = -(2\pi)^{-2} \left(\sqrt{\pi}e^{-\rho^2/4} + \frac{\pi}{\rho} \text{erfc}(\rho/2)\right),$$

where $\text{erfc} = 1 - \text{erf}$. We could decide to use $s(|x|/ah)$ instead of $s(|x|/h)$ in the definition of G_h , where $a > 0$ is some constant. The effect would be to replace G_h by G_{ah} . Then $(G_1 \circ J)$ would be replaced by $(G_a \circ J)$, and (2.17) by

$$(2.25) \quad (G_a \circ J)^\wedge(k) = a(\det g_{\mu\nu})^{-1/2} \Gamma(a\rho), \quad \rho = \sqrt{g^{\mu\nu}k_\mu k_\nu}.$$

The condition $\hat{G}_h < 0$ is evident in (2.22) for the specific choice of G_h given by (2.19). The condition would hold for a variety of other choices as well. Suppose we first choose a smooth delta function as in (2.6) by taking $\psi_{(1)}$ to be a smooth, rapidly decreasing, radial function, with integral one, such that $\hat{\psi}_{(1)}(k) > 0$ and $\hat{\psi}_{(1)}$ decreases with $|k|$. If we define $s_{(1)}$ by (2.5), $s_{(3)}$ by (2.10), and G_h by (2.1) using $s_{(3)}$, it follows that the needed conditions hold, including $\hat{G}_h < 0$.

We next discuss the periodic versions of the Green’s function and its regularization. Because of the slow decay at infinity, we write the sum with a reflection and with a constant subtracted from each term. We define

$$(2.26) \quad G^\pi(x) = \frac{1}{2} \sum'_{n \in \mathbf{Z}^2} \left(G(x - 2\pi(n, 0)) + G(x + 2\pi(n, 0)) + \frac{1}{2\pi|n|} \right),$$

where the prime on the sum means that $1/|n|$ is omitted at $n = 0$. The gradient is

$$(2.27) \quad \nabla G^\pi(x) = \frac{1}{2} \sum_{n \in \mathbf{Z}^2} (\nabla G(x - 2\pi(n, 0)) + \nabla G(x + 2\pi(n, 0))),$$

and we define $G_h^\pi, \nabla G_h^\pi$ similarly.

Lemma 2.1. *The sums for $G_h^\pi(x)$ and $\nabla G_h^\pi(x)$ converge uniformly on bounded sets for fixed h , and those for $G^\pi(x)$ and $\nabla G^\pi(x)$ converge in L^1 on bounded sets. $G^\pi(x)$ and $G_h^\pi(x)$ are periodic and satisfy*

$$(2.28) \quad \Delta G^\pi(x) = \sum_n \delta(x + 2\pi(n, 0)), \quad \Delta G_h^\pi(x) = \sum_n \psi_h(x + 2\pi(n, 0)).$$

Proof. For fixed x and large y , we have

$$(2.29) \quad G(x + y) = -\frac{1}{4\pi} \left(\frac{1}{|y|} - \frac{y \cdot x}{|y|^3} + O(|y|^{-3}) \right) \quad \text{as } y \rightarrow \infty.$$

If we add $G(x \pm y)$, the second term above is canceled, and so with $y = \pm 2\pi(n, 0)$, we see that the n th term in (2.26) is $O(|n|^{-3})$. Thus the sum for $G^\pi(x)$ converges pointwise away from the singularity, and since the singularity is integrable, the sum also converges in L^1 on a bounded set. For the regularized version G_h , we note that

$$(2.30) \quad |G_h(x \pm 2\pi(n, 0)) - G(x \pm 2\pi(n, 0))| = O(|n|^{-5}) \quad \text{as } n \rightarrow \infty$$

because of (2.2). Thus the sum for G_h^π converges similarly to G^π , but G_h^π is bounded for fixed h , so that the convergence is uniform on bounded sets. It is correct to apply Δ termwise in the distributional sense, so that both equations (2.28) hold as distributions. However, since ΔG_h^π is smooth, the second case is true in the classical sense as well. Similar considerations apply to the gradients.

It remains to verify that G^π and G_h^π are actually periodic. Specifically, let x be a point which is not a periodic image of 0; we verify that $G^\pi(x + (2\pi, 0, 0)) = G^\pi(x)$. We will use the notation $r(n) = |n|^{-1}$ if $n \neq 0$, $r(0) = 0$, and also $n^+ = (n_1 + 1, n_2, 0)$, $n^- = (n_1 - 1, n_2, 0)$. Let $B_M = \{(n_1, n_2) \in \mathbf{R}^2 : |n_j| \leq M, j = 1, 2\}$. Then

$$(2.31) \quad -8\pi G^\pi(x + (2\pi, 0, 0)) = \lim_{M \rightarrow \infty} \sum_{B_M} (|x + 2\pi n^+|^{-1} + |x - 2\pi n^-|^{-1} - 2r(n)).$$

We will show below that we can replace $2r(n)$ above by $r(n^+) + r(n^-)$. If we do this, the sum over B_M can be rewritten as

$$(2.32) \quad \sum_{B_M} (|x + 2\pi n^+|^{-1} - r(n^+)) + \sum_{B_M} (|x - 2\pi n^-|^{-1} - r(n^-)).$$

In the first sum we can shift the n^+ back to n , ranging over B_M , except for $O(M)$ terms, each of size $O(M^{-2})$. Since B_M is symmetric, $n \rightarrow -n$, this sum converges

to $-4\pi G^\pi(x)$ as $M \rightarrow \infty$. The same argument applies to the n^- term, and the desired equality is verified. The same argument works for G_h^π .

We still must show that the replacement above did not change (2.31); i.e., we must show that the absolutely convergent sum $\sum (r(n^+) + r(n^-) - 2r(n))$ is zero. It is the limit as $M \rightarrow \infty$ of

$$(2.33) \quad \sum_{B_M} (r(n^+) - r(n)) + \sum_{B_M} (r(n^-) - r(n)) .$$

We can shift the index in the second sum and write it as the sum of $r(n) - r(n^+)$ over a set which is B_M , except for $O(M)$ terms each of size $O(M^{-2})$. Within B_M , the terms cancel exactly, and therefore the expression above approaches 0 as $M \rightarrow \infty$. □

Finally we estimate the error introduced by the regularization of the Green's function for single or double layer potentials on a doubly periodic surface.

Theorem 2.2. *Let $\alpha \rightarrow x$ be a smooth mapping from \mathbf{R}^2 to \mathbf{R}^3 so that $x(\alpha) - (\alpha, 0)$ is doubly periodic with period 2π and (1.13) is satisfied. Let f be a smooth periodic function of α , G^π the periodic Green's function, and G_h^π the regularized version. Then for any α_0*

$$(2.34) \quad \left| \int G_h^\pi(x(\alpha_0) - x(\alpha))f(\alpha) d\alpha - \int G^\pi(x(\alpha_0) - x(\alpha))f(\alpha) d\alpha \right| \leq Ch^3,$$

where the integral is over a period square in α .

Proof. We can take the domain of integration to be

$$(2.35) \quad B_0 = \{ \alpha = (\alpha_1, \alpha_2) \in \mathbf{R}^2 : |\alpha_\nu - (\alpha_0)_\nu| < \pi, \nu = 1, 2 \} .$$

To separate out the singularity, we introduce a cut-off function ζ on \mathbf{R}^2 so that $\zeta(\alpha) = 1$ near $\alpha = 0$ and $\zeta(\alpha) = 0$ for $|\alpha| > \pi/2$. Now define, for all α ,

$$(2.36) \quad G_{h0}^\pi(\alpha) = \sum_{n \in \mathbf{Z}^2} G_h(x(\alpha_0) - x(\alpha) - 2\pi(n, 0))\zeta(\alpha_0 - \alpha - 2\pi n) .$$

Then G_{h0}^π is periodic in α , since adding a period to α only shifts the sum; only one term can be nonzero. Similarly we define G_0^π from G^π using the same ζ . Let $G_{h\infty}^\pi = G_h^\pi - G_{h0}^\pi$ and $G_\infty^\pi = G^\pi - G_0^\pi$, as functions of α . Now $G_{h\infty}^\pi$ and G_∞^π are smooth and periodic. We first argue that their difference contributes little to the integral. From (2.2), we have

$$(2.37) \quad |G_h(x(\alpha_0) - x(\alpha)) - G(x(\alpha_0) - x(\alpha))| \leq Ch^4|x(\alpha_0) - x(\alpha)|^{-5}$$

provided $|x(\alpha_0) - x(\alpha)|$ is bounded away from zero. By (1.13), the latter is true if $|\alpha_0 - \alpha|$ is bounded away from zero, as it is on the support of $1 - \zeta$. The same is true with α replaced by $\alpha + 2\pi n$. Consequently $G_{h\infty}^\pi - G_\infty^\pi$ is $O(h^4)$, uniformly in α ; the n th term decays like $|n|^{-5}$, so that the sum of estimates converges. Thus the integral corresponding to the difference $G_{h\infty}^\pi - G_\infty^\pi$ is also $O(h^4)$. We are now reduced to the case where G_h^π and G^π are replaced by G_{h0}^π and G_0^π . We note that for $\alpha \in B_0$ we have $|\alpha_0 - \alpha \pm 2\pi n| > \pi$ for $n \neq 0$, so that $\zeta = 0$ there. Consequently $G_{h0}^\pi(\alpha) = G_h(x(\alpha_0) - x(\alpha))\zeta(\alpha_0 - \alpha)$ for $\alpha \in B_0$, and similarly for G_0^π .

It remains to obtain a local estimate near the singularity at α_0 . For convenience we assume from now on that $\alpha_0 = 0$ and $x(\alpha_0) = 0$. We also may as well assume

that $f(\alpha)$ has support near $\alpha = 0$, because of the ζ factor. The proof now amounts to showing that

$$(2.38) \quad \left| \int_{\mathbf{R}^2} (G_h(x(\alpha)) - G(x(\alpha))) f(\alpha) d\alpha \right| \leq Ch^3.$$

The integral is

$$(2.39) \quad - \int_{\mathbf{R}^2} (s(r/h) - 1) \left(\frac{1}{4\pi r} \right) f(\alpha) d\alpha, \quad r = |x(\alpha)|.$$

Let (ρ, θ) be polar coordinates for α ; the integral becomes

$$(2.40) \quad -(4\pi)^{-1} \int_0^{2\pi} \int_0^\infty (s(r/h) - 1) \frac{\rho}{r} f(\alpha) d\rho d\theta.$$

We will change variables in the inner integral from ρ to r . First we write the Taylor formula for $x(\alpha)$ as $x(\alpha) = J\alpha + q(\alpha) + O(\alpha^3)$, where $J = (\partial x/\partial \alpha)(0)$ and q is bilinear. As a consequence we can write

$$(2.41) \quad r/\rho = |x(\alpha)|/|\alpha| = a(\theta) + b(\theta)\rho + \gamma(\rho, \theta)\rho^2,$$

where γ is smooth in (ρ, θ) , regarded as independent variables. Here

$$(2.42) \quad a(\theta) = |J\alpha|/|\alpha|, \quad b(\theta) = J\alpha \cdot q(\alpha)/|\alpha|^2 |J\alpha|.$$

For later use we note that a is even and b is odd in α , i.e., $a(\theta + \pi) = a(\theta)$, $b(\theta + \pi) = -b(\theta)$. Assuming the support of the cut-off function ζ was chosen small enough, we can invert (2.41) to obtain

$$(2.43) \quad \rho/r = \tilde{a}(\theta) + \tilde{b}(\theta)r + \tilde{\gamma}(r, \theta)r^2,$$

where $\tilde{a} = 1/a$, $\tilde{b} = -b/a^3$, so that \tilde{a}, \tilde{b} have the same parity as a, b , and $\tilde{\gamma}(r, \theta)$ is smooth. We now convert the ρ -integral above to

$$(2.44) \quad \int_0^\infty (s(r/h) - 1) \frac{\rho}{r} \frac{\partial \rho}{\partial r} f(\alpha) dr.$$

Only the low powers of r will matter, and we use Taylor expansions. We have $\rho/r = \tilde{a} + \tilde{b}r + O(r^2)$ and $\partial \rho/\partial r = \tilde{a} + 2\tilde{b}r + O(r^2)$. We can write the expression for $f(\alpha)$ as $f = f_0 + f_1(\theta)\rho + O(\rho^2)$, with $f_1(\theta)$ odd. Converting from ρ to r , we have $f = f_0 + \tilde{a}f_1r + O(r^2)$. Multiplication of these expressions gives

$$(2.45) \quad (\rho/r)(\partial \rho/\partial r)f(\alpha) = \tilde{a}^2 f_0 + (3\tilde{a}\tilde{b}f_0 + \tilde{a}^3 f_1)r + \tilde{f}(r, \theta)r^2$$

with \tilde{f} smooth in r, θ . When we substitute this into the integral, the constant term contributes zero because of the moment condition (2.9). The term linear in r has a coefficient which is odd, so that it also contributes zero after integration in θ . The remaining part of the r -integral is now

$$(2.46) \quad \int_0^\infty (s(r/h) - 1) \tilde{f}(r, \theta)r^2 dr = h^3 \int_0^\infty (s(r/h) - 1) \tilde{f}(r, \theta)(r/h)^2 d(r/h).$$

The last integral is bounded uniformly in h , since \tilde{f} is bounded and $s - 1$ decreases rapidly. The total error has been reduced to the last expression and is therefore $O(h^3)$, as claimed. □

Next we have the analogue of Theorem 2.2 for double layer potentials.

Theorem 2.3. *Let $\alpha \rightarrow x$ be the mapping of Theorem 2.2, and let $F(\alpha)$ be a smooth vector-valued function of α . Assume that for some α_0 the vector $F(\alpha_0)$ is parallel to n_0 , the normal to the surface at $x(\alpha_0)$. Then*

$$(2.47) \quad \left| \int \nabla G_h^\pi(x(\alpha_0) - x(\alpha)) \cdot F(\alpha) \, d\alpha - \int \nabla G^\pi(x(\alpha_0) - x(\alpha)) \cdot F(\alpha) \, d\alpha \right| \leq Ch^3,$$

where the integral is over a period square in α .

Proof. As in Theorem 2.2, we can reduce the estimate to the case where $\alpha_0 = 0$, $x(\alpha_0) = 0$, and F is supported in a small neighborhood of $\alpha = 0$. We then need to show that

$$(2.48) \quad \left| \int_{\mathbf{R}^2} (\nabla G_h(x(\alpha)) - \nabla G(x(\alpha))) \cdot F(\alpha) \, d\alpha \right| \leq Ch^3.$$

The integral is proportional to

$$(2.49) \quad \int_{\mathbf{R}^2} (\tilde{s}(r/h) - 1) r^{-3} x(\alpha) \cdot F(\alpha) \, d^2\alpha, \quad r = |x(\alpha)|.$$

Proceeding as before, we obtain the r -integral

$$(2.50) \quad \int_0^\infty (\tilde{s}(r/h) - 1) x(\alpha) \cdot F(\alpha) r^{-3} \rho \frac{\partial \rho}{\partial r} \, dr.$$

Expanding x as $x(\alpha) = J\alpha + q(\alpha) + O(\rho^3)$ and $F(\alpha) = F_0 + F_1\rho + O(\rho^2)$, and noting that $J\alpha \cdot F_0 = 0$, we have

$$(2.51) \quad x \cdot F(\alpha) = c_2(\theta)\rho^2 + c_3(\theta)\rho^3 + O(\rho^4)$$

with c_2 even and c_3 odd. Now using $\rho = \tilde{a}r + \tilde{b}r^2 + O(r^3)$, we get

$$(2.52) \quad x \cdot F = c_2\tilde{a}^2r^2 + (c_3\tilde{a}^3 + 2\tilde{a}\tilde{b})r^3 + O(r^4).$$

Multiplying out, we find that

$$(2.53) \quad (x \cdot F)r^{-3}\rho(\partial\rho/\partial r) = \tilde{a}^4c_2 + (\tilde{a}^5c_3 + 2\tilde{a}^3\tilde{b}c_2 + 3\tilde{a}^3\tilde{b}c_2)r + O(r^2).$$

The coefficient of r is odd, and the argument proceeds just as before. □

3. QUADRATURE OF SINGULAR INTEGRALS

In this section we develop a general approach to quadrature for singular integrals with regularization. We find an expansion in powers of h for the error in the trapezoidal rule, similar to that of Lyness [23] and Goodman et al. [12] without regularization, adapting the approach of [12]. We show that the largest error can be identified in terms of the Fourier transform of the regularized kernel using the Poisson summation formula. A correction can then be found to improve the order of accuracy. The application to single and double layer potentials is given in Theorem 3.7. We derive the correction terms in (1.26), (1.27) and prove that the quadrature errors in these equations are $O(h^3)$. For unregularized singular integrals, corrections are more difficult to find, but methods have been developed in [22], [17].

For later reference, we state the Poisson summation formula for a smooth, rapidly decreasing function f on \mathbf{R}^d :

$$(3.1) \quad (2\pi)^{-d/2} \sum_{j \in Z^d} f(jh) e^{-ikjh} h^d = \sum_{n \in Z^d} \hat{f}(k + 2\pi n/h)$$

We will need a general estimate for quadrature of mildly regular functions. The following statement was proved in [11], [1] for F independent of h . The proof of Lemma 2.2 in [1] is direct from the Poisson formula.

Lemma 3.1. *Let $F(x)$ be a function of x in \mathbf{R}^d such that $D_x^\beta F$ is in $L^1(\mathbf{R}^d)$ for multi-indices β with $|\beta| = \ell$, where $\ell \geq d + 1$. Then, with a universal constant C_ℓ ,*

$$(3.2) \quad \left| \sum_{n \in \mathbf{Z}^d} F(nh) h^d - \int_{\mathbf{R}^d} F(x) dx \right| \leq C_\ell h^\ell \sum_{|\beta|=\ell} |D_x^\beta F|_{L^1}.$$

We begin with a treatment of quadrature errors for singular integrals, regularized on the scale of the grid size. We start with a singular kernel $K(x)$, defined for nonzero x in d -space \mathbf{R}^d , which is homogeneous of degree m for integer m , i.e.,

$$(3.3) \quad K(ax) = a^m K(x), \quad a > 0, \quad x \neq 0.$$

We also work with modified kernels of the form $K_h(x) = K(x)s(x/h)$, where s approaches 1 for large argument, and s is chosen so that K_h is smooth up to $x = 0$. Note that $K_h(x) = h^m K_1(x/h)$. The following two lemmas will be fundamental. They are adapted from the proof of Lemma 1 in [12].

Lemma 3.2. *Let K and s be smooth functions on $\mathbf{R}^d - \{0\}$ such that K is homogeneous of degree m , in the sense of (3.3), and*

$$(3.4) \quad |D^k s(x)| \leq C|x|^{-|k|}, \quad |x| \geq 1.$$

For $h > 0$, let $K_h(x) = K(x)s(x/h)$, and assume K_h continues as a smooth function to $x = 0$, so that $K_h(0) = h^m K_1(0)$. Finally, let $\zeta(x)$ be a smooth cut-off function with $\zeta(x) \equiv 1$ for x in a neighborhood of 0 and $\zeta = 0$ outside a bounded set. Now approximate the integral

$$(3.5) \quad I = \int_{\mathbf{R}^d} K_h(x)\zeta(x) dx = \int_{\mathbf{R}^d} K(x)s(x/h)\zeta(x) dx$$

by the sum of values at nh , where n is a multi-integer:

$$(3.6) \quad S = \sum_{n \in \mathbf{Z}^d} K_h(nh)\zeta(nh)h^d = \sum_{n \in \mathbf{Z}^d} K(nh)s(n)\zeta(nh)h^d.$$

Then as $h \rightarrow 0$,

$$(3.7) \quad S - I = c_0 h^{d+m} + O(h^\ell),$$

where ℓ is large depending on the smoothness of $K(x)$ and $s(x)$ for $|x| \geq 1$.

For example, if $m = 1 - d$, we have a first order error with a much smaller remainder. In some cases we can identify the constant c_0 , as explained below. In the second expression for the sum S , the proper limiting value should be used for the $n = 0$ term, namely $K_1(0)h^{d+m}$. The proof of the lemma below also shows that the quadrature error for the unmodified K , omitting the $n = 0$ term, has the same behavior in case $m \geq 1 - d$, as shown in [12]:

$$(3.8) \quad \sum_{n \neq 0} K(nh)\zeta(nh)h^d - \int_{\mathbf{R}^d} K(x)\zeta(x) dx = c'_0 h^{d+m} + O(h^\ell).$$

In the regularized case, the $n = 0$ term is $O(h^{d+m})$, so that the conclusion is valid whether or not the $n = 0$ term is included in the quadrature.

Proof. We use a simplified version of the argument in [12], modified for the smoothing of the kernel. We can rewrite the integral I using the substitution $y = x/h$ and the homogeneity of K as

$$(3.9) \quad I = h^{d+m}\mathcal{I}, \quad \mathcal{I} \equiv \int_{\mathbf{R}^d} K(y)s(y)\zeta(yh) dy.$$

Similarly we can write the sum as

$$(3.10) \quad S = h^{d+m}\mathcal{S}, \quad \mathcal{S} \equiv \sum_n K(n)s(n)\zeta(nh).$$

Now h appears inside \mathcal{I} and \mathcal{S} only in ζ . As in [12] we differentiate in h and compare the resulting sum and integral. We find that

$$\mathcal{I}'(h) = \int_{\mathbf{R}^d} K(y)s(y) y \cdot \nabla\zeta(yh) dy = h^{-(d+m+1)} \int_{\mathbf{R}^d} K(x)s(x/h) x \cdot \nabla\zeta(x) dx$$

and

$$\mathcal{S}'(h) = \sum_n K(n)s(n) n \cdot \nabla\zeta(nh) = h^{-(d+m+1)} \sum_n K(nh)s(n) (nh) \cdot \nabla\zeta(nh) \cdot h^d.$$

The integrand and summand are nonzero only on the support of $\nabla\zeta$. We take this support to be $\{x : r_1 \leq |x| \leq r_2\}$ for some $r_2 > r_1 > 0$. We can regard the last sum as a trapezoidal rule approximation to the integral above. To estimate the error using Lemma 3.1 we need to estimate the derivatives of the integrand. Since $|x| \geq r_1$, derivatives of K are uniformly bounded. Moreover, from 3.4 we have

$$(3.11) \quad |D_x^k(s(x/h))| \leq C|x|^{-|k|}, \quad |x| \geq h.$$

Thus the L^1 norm of each derivative of the integrand is bounded uniformly in h , up to some order limited by the smoothness of K and s . Then, by Lemma 3.1,

$$(3.12) \quad |\mathcal{S}'(h) - \mathcal{I}'(h)| \leq C_\ell h^{\ell-d-m-1}, \quad h > 0,$$

for large ℓ . Now $\mathcal{S}(h) - \mathcal{I}(h)$ is smooth for $h > 0$ and has a limit at $h = 0$ provided ℓ is large enough. Then

$$(3.13) \quad (\mathcal{S} - \mathcal{I})(h) = (\mathcal{S} - \mathcal{I})(0) + \int_0^h (\mathcal{S}' - \mathcal{I}') = c_0 + O(h^{\ell-d-m})$$

for some constant c_0 , so that $S(h) - I(h) = c_0 h^{d+m} + O(h^\ell)$, as claimed. □

Lemma 3.3. *Let K, s, K_h, m, ζ be as in the previous lemma, and let $f(x)$ be a smooth function on \mathbf{R}^d such that f and its derivatives are rapidly decreasing. Assume that K, s and ζ are even in x . Then the integral*

$$(3.14) \quad I = \int_{\mathbf{R}^d} K_h(x)f(x) dx = \int_{\mathbf{R}^d} K(x)s(x/h)f(x) dx$$

is approximated by the sum

$$(3.15) \quad S = \sum_{n \in \mathbf{Z}^d} K_h(nh)f(nh)h^d = \sum_{n \in \mathbf{Z}^d} K(nh)s(n)f(nh)h^d.$$

with error

$$(3.16) \quad S - I = h^{d+m} (c_0 f(0) + C_2 h^2 + \dots + C_{2\ell} h^{2\ell} + O(h^{2\ell+2})),$$

where c_0 is as in (3.7) and C_2 etc. depend on g . If K is odd and s is even, we have a similar expansion but with h^{d+m} replaced by h^{d+m+1} , and the leading error is proportional to $\nabla f(0)$.

Proof. The error from $(1 - \zeta)f$ is easily seen to be high order. For ζf we use a second order Taylor expansion for f , multiplied by ζ ,

$$(3.17) \quad \zeta(x)f(x) = f(0)\zeta(x) + (\nabla f(0) \cdot x)\zeta(x) + \tilde{f}(x),$$

where \tilde{f} is a remainder of compact support. The constant term in f leads to an integral whose quadrature error is the first term above plus a higher order part, according to the preceding lemma. The linear term in f leads to an integrand which is odd in x , provided K and s are even; thus the integral for this term is zero, and the same is true for the sum, since the grid respects the symmetry.

Next we estimate the quadrature error coming from $\tilde{f}(x)$. The remainder \tilde{f} consists of a sum of terms, each of the form $\gamma(x)b(x)$, where b is bilinear and γ is smooth. The integrand arising from such a term is

$$(3.18) \quad F(x; h) = K(x)s(x/h)b(x)\gamma(x) = h^{m+2}g(x/h)\gamma(x),$$

where g is the smooth function $Ksb = K_1b$. In order to apply Lemma 3.1, we estimate x -derivatives of F . Now from the assumption (3.4) on s and the homogeneity of K we have $|D_x^k g(x)| \leq |x|^{m+2-k}$, so that

$$(3.19) \quad |D_x^k F(x; h)| \leq C|x|^{m+2-k}, \quad |x| \geq h, \quad k \geq 0.$$

On the other hand, for $|x| \leq h$, we can use the smoothness of K_1 to estimate

$$(3.20) \quad |D_x^k F(x; h)| \leq Ch^{m+2-k}, \quad |x| \leq h, \quad k \geq 0.$$

Combining these two pointwise estimates and integrating, we get

$$(3.21) \quad |D_x^k F|_{L^1} \leq Ch^{m+2+d-k}.$$

Lemma 3.1 now implies that the quadrature error is $O(h^{m+2+d})$, and we have proved (3.16) with $\ell = 0$.

The expansion can be carried further in the same way, as allowed by the smoothness, with zero contribution from the odd order terms in the Taylor series for f by symmetry. If K is odd rather than even, the sum and integral from the even terms in the Taylor series drop out, beginning with the constant $f(0)$. \square

Lemma 3.4. *With K and K_h as in Lemmas 3.2 and 3.3, the constant c_0 in (3.7), (3.16) is given by*

$$(3.22) \quad c_0 = (2\pi)^{d/2} \sum_{n \neq 0} \hat{K}_1(2\pi n)$$

Proof. The hypothesis on K_h implies that $D^j K_1$ is in $L^1(\mathbf{R}^d)$ for j large; consequently $\hat{K}_1(k)$ and its derivatives decrease rapidly for $k \neq 0$. We use Lemma 3.3 with a convenient choice of f . Suppose $f(0) = 1$. Then, from (3.16) and (3.3),

$$(3.23) \quad c_0 = \lim_{h \rightarrow 0} h^{-(m+d)}(S - I) = \lim_{h \rightarrow 0} \left(\sum K_1(n)f(nh) - \int K_1(y)f(yh) dy \right).$$

We choose f so that $\hat{f}(k)$ is smooth everywhere and zero outside $|k| \leq 1$. Now let $F_h(x) = K_1(x)f(xh)$. Then F_h is smooth and rapidly decreasing, and we can apply the Poisson summation formula (with $k = 0, h = 1$ in (3.1)) to obtain

$$(3.24) \quad c_0 = \lim_{h \rightarrow 0} (2\pi)^{d/2} \sum_{n \neq 0} \hat{F}_h(2\pi n).$$

We need to justify passage to the limit to obtain (3.22). Since F_h is a product, \hat{F}_h is the convolution of \hat{K}_1 with $(2\pi)^{-d/2}h^{-d}\hat{f}(k/h)$, an approximate delta function. We can write $\hat{F}_h(k) - \hat{K}_1(k)$ as an integral and show by a standard argument, using the compact support of \hat{f} and the decay of $D\hat{K}_1$, that $|\hat{F}_h(k) - \hat{K}_1(k)| \leq Ch|k|^{-d-1}$ for $k \geq 1$. Thus the sum in (3.24) tends to the sum with \hat{K}_1 in place of \hat{F}_h . \square

We now apply the above lemmas to determine quadrature errors for single or double layer potentials on a doubly periodic surface, using the regularized Green's function of (2.1). We first deal with the neighborhood of the singularity. For convenience we place the singularity at zero in both α and x coordinates. Recall that $G_h(x)$ is a smooth function of x the form $r^{-1}s(r/h)$, $r = |x|$, and $G_h(x) = h^{-1}G_1(x/h)$.

Lemma 3.5. *Let $\alpha \rightarrow x$ be a smooth mapping from a neighborhood U of 0 in \mathbf{R}^2 into \mathbf{R}^3 , with $0 \rightarrow 0$. Let J be the Jacobian matrix $(\partial x/\partial \alpha)(0)$, so that $x = J\alpha + O(\alpha^2)$. Assume that J has full rank and U is small enough so that*

$$(3.25) \quad |J\alpha|/2 \leq |x| \leq 2|J\alpha|, \quad \alpha \in U.$$

Let G_h be a regularized Green's function obeying (2.1)–(2.3), and let $f(\alpha)$ be a smooth function with support in U . Then as $h \rightarrow 0$

$$(3.26) \quad \sum_{n \in \mathbf{Z}^2} G_h(x(nh))f(nh)h^2 - \int_U G_h(x(\alpha))f(\alpha) d\alpha = c_0f(0)h + O(h^3),$$

where

$$(3.27) \quad c_0 = 2\pi \sum_{n \neq 0} (G_1 \circ J)^\wedge(2\pi n),$$

or, with Γ as in (2.14), $g_{\mu\nu} = (J^*J)_{\mu\nu}$, and $g^{\mu\nu}$ the inverse,

$$(3.28) \quad c_0 = 2\pi(\det g_{\mu\nu})^{-1/2} \sum_{n \neq 0} \Gamma(2\pi\sqrt{g^{\mu\nu}n_\mu n_\nu}).$$

Proof. Since G_1 is a smooth function of x , it is a smooth function of $|x|^2$, i.e., we can write $G_1(x) = g(|x|^2)$ for a smooth function g of one variable, and therefore $G_h(x) = h^{-1}g(\rho^2)$, where $\rho = |x|/h$. For later use we note that the decay assumption (2.2) for s implies that

$$(3.29) \quad |D^k g(\sigma)| \leq C|\sigma|^{-(k+1/2)}, \quad |\sigma| \geq 1.$$

We want to relate the composition $G_h(x(\alpha))$ to the simpler case where $x(\alpha)$ is replaced by $J\alpha$, a case to which the earlier lemmas apply. To this end we use a Taylor expansion for g as a function of ρ^2 about ρ_1^2 , and then set $\rho = |x(\alpha)|/h$ and $\rho_1 = |J\alpha|/h$:

$$(3.30) \quad g(\rho^2) = g(\rho_1^2) + g'(\rho_1^2)(\rho^2 - \rho_1^2) + \tilde{g}(\rho_1, \rho)(\rho^2 - \rho_1^2)^2,$$

with some smooth \tilde{g} . Further, we can write $x(\alpha)$ in a Taylor expansion about $\alpha = 0$, beginning with $J\alpha$, to obtain

$$(3.31) \quad \rho^2 - \rho_1^2 = h^{-2}(p_3(\alpha) + y(\alpha)),$$

where p_3 is trilinear in α and the remainder y has degree 4 or higher. Combining these, we have an expansion of G_h in terms with successively higher homogeneity

in α and h together; we write $G_h = G_h^{(-1)} + G_h^{(0)} + G_h^{(1)}$, as a function of α , where

$$(3.32) \quad G_h^{(-1)} = h^{-1}g(\rho_1^2) = G_h(J\alpha) = -(4\pi|J\alpha|)^{-1}s(|J\alpha|/h),$$

$$(3.33) \quad G_h^{(0)} = h^{-3}g'(\rho_1^2)p_3(\alpha),$$

with nonhomogeneous remainder

$$(3.34) \quad G_h^{(1)} = h^{-3}g'(\rho_1^2)y + h^{-1}\tilde{g}(\rho_1, \rho)(\rho^2 - \rho_1^2)^2.$$

We multiply the expanded integrand by a cut-off function $\zeta(\alpha)$ which is even and equals 1 on the support of f , and assess the quadrature errors from the various terms. For the leading term $G_h^{(-1)}$, we have the integrand $G_h(J\alpha)f(\alpha)\zeta(\alpha)$. Lemma 3.3 applies with $m = -1$ and x, K_h replaced by $\alpha, G_h \circ J$. Recalling (2.17), we obtain the first order error term as stated. For the next term we note that p_3 is odd in α and ρ_1^2 is even, so that $G_h^{(0)}(\alpha)$ is odd, and the contribution from $f(0)$ drops out. Using Lemma 3.3, we see that the error from $G_h^{(0)}(\alpha)f(\alpha)\zeta(\alpha)$ is $O(h^3)$.

Finally we verify that the quadrature error resulting from $G_h^{(1)}$ is $O(h^3)$, considering the two terms separately. The remainder y in (3.31) is a sum of terms of the form $\tilde{y}(\alpha)p_4(\alpha)$, where p_4 is homogeneous of degree 4 and \tilde{y} is smooth. Thus by Lemma 3.3 the integrand $h^{-3}g'(\rho_1^2)\tilde{y}(\alpha)p_4(\alpha)$ has quadrature error $O(h^{-3+4+2}) = O(h^3)$. For the last term we need to estimate directly. The remainder \tilde{g} in g is

$$(3.35) \quad \tilde{g}(\rho_1, \rho) = \int_0^1 tg''(t\rho_1^2 + (1-t)\rho^2) dt.$$

Using (3.29) and (3.25), we can conclude that

$$(3.36) \quad |D_\alpha^k \tilde{g}(\rho_1, \rho)| \leq Ch^5 |\alpha|^{-(5+k)}, \quad |\alpha| \geq c_1h,$$

with c_1 a constant large enough so that $|\alpha| \geq c_1h$ implies $|x| \geq h$. We can write $\rho^2 - \rho_1^2$ as a sum of terms of the form $h^{-2}q_3(\alpha)r(\alpha)$, where q_3 is trilinear. Thus the last term in (3.34) leads to the integrand $F(\alpha) = h^{-5}\tilde{g}(\rho_1, \rho)q_3(\alpha)^2r(\alpha)^2\zeta(\alpha)$. We estimate the quadrature error using Lemma 3.1. Using (3.36), we find that

$$(3.37) \quad |D^k F(\alpha)| \leq C|\alpha|^{1-k}, \quad |\alpha| \geq c_1h.$$

On the other hand, for $|\alpha| \leq c_1h$, we have $|D_\alpha^k \tilde{g}| = O(h^{-k})$, and consequently

$$(3.38) \quad |D^k F(\alpha)| \leq Ch^{1-k}, \quad |\alpha| \leq c_1h.$$

Combining these two pointwise estimates, we have $|D^k F|_{L^1} \leq Ch^{3-k}$, and by Lemma 3.1 the quadrature error is $O(h^3)$. □

The next lemma concerns the double layer potential near the singularity. We recall that the gradient of the regularized Green's function, ∇G_h , has the form $r^{-3}x\tilde{s}(|x|/h)$. We assume it is multiplied by a vector-valued function $F(\alpha)$ which is normal at the singular point, so that the product is integrable.

Lemma 3.6. *Assume the mapping $\alpha \rightarrow x$, the set U , and the function G_h are as in Lemma 3.5. Let $F(\alpha)$ be a smooth vector-valued function with support in U such that $F(0)$ is parallel to n_0 , the unit normal to the surface $x(\alpha)$ at $x(0) = 0$. Then*

$$(3.39) \quad \sum_{n \in \mathbf{Z}^2} \nabla G_h(x(nh)) \cdot F(nh)h^2 - \int_U \nabla G_h(x(\alpha)) \cdot F(\alpha) d\alpha = C_0h + O(h^3),$$

for some C_0 depending on F . In particular, $C_0 = 0$ and the error is $O(h^3)$ under the stronger assumption

$$(3.40) \quad F(\alpha) \cdot n_0 = O(\alpha) \quad \text{and} \quad F^T(\alpha) = O(\alpha^2) \quad \text{as} \quad \alpha \rightarrow 0,$$

where $F^T(\alpha)$ is the projection of $F(\alpha)$ orthogonal to n_0 .

Proof. We use an argument like the proof of Lemma 3.5. The function \tilde{s} in ∇G_h (cf. (2.11)) has the form $\tilde{s}(\rho) = \rho^3 g(\rho^2)$, where g is a smooth function, so that

$$(3.41) \quad \nabla G_h(x) = h^{-3} g(\rho^2) x, \quad \rho = |x|/h.$$

Let $x(\alpha) = x_1(\alpha) + x_2(\alpha) + \dots$ be the Taylor expansion for $x(\alpha)$ about $\alpha = 0$, with $x_1 = J\alpha$ linear, x_2 bilinear, etc. As in (3.30) we expand $g(\rho^2)$ about ρ_1^2 , with $\rho_1 = |x_1|/h$, and substitute for $\rho^2 - \rho_1^2$ in terms of the x 's. We collect terms according to degree in α, h together. In this way we write $\nabla G_h = K_{-2} + K_{-1} + K_0 + K_1 + \dots$ as functions of α . The first two are

$$(3.42) \quad K_{-2} = h^{-3} g(\rho_1^2) x_1,$$

$$(3.43) \quad K_{-1} = h^{-3} g(\rho_1^2) x_2 + 2h^{-5} g'(\rho_1^2) (x_1 \cdot x_2) x_1.$$

We consider first the quadrature of $K_{-2}(\alpha) \cdot F(\alpha)$. (As usual we multiply by a cut-off covering the support of F .) The term $K_{-2}(\alpha) \cdot F(0)$ is zero, since $x_1(\alpha)$ is tangent and $F(0)$ is normal by hypothesis. Then Lemma 3.3 implies that the quadrature error has the form $C_0 h + O(h^3)$, with C_0 determined by the scalar product of $x_1(\alpha)$ with the linear term in the expansion of F . Under the hypothesis (3.40), this linear term is parallel to n_0 , so that the $O(h)$ error vanishes. For K_{-1} , we again have an error of the form $Ch + O(h^3)$, according to Lemma 3.3. The $O(h)$ term comes from the constant $F(0)$, and it vanishes under hypothesis (3.40). It can be seen that K_0 is odd in α , so that by Lemma 3.3 it contributes an error $O(h^3)$. Similar considerations show that higher order terms beyond K_0 lead to errors $O(h^3)$ or smaller. To obtain terms up to K_0 , we need to expand g to the second order, x to the third order, and $\rho^2 - \rho_1^2$ to the fourth degree terms, all with remainders. Finally, we can estimate the quadrature errors due to the remainders, in a manner similar to Lemma 3.5, and show that they are $O(h^3)$. The remainder in $g(\rho^2)$ has the form $\tilde{g}(\rho, \rho_1)(\rho^2 - \rho_1^2)^3$, where \tilde{g} is an average of g''' . In this case $g(\rho^2)$ decays like ρ^{-3} , and the assumptions on the decay of \tilde{s} imply that $|D_\alpha^k \tilde{g}(\rho, \rho_1)| \leq C|\alpha|^{-(9+k)}$ for $|\alpha| \geq c_1 h$. Otherwise the treatment of this term proceeds as before. \square

Now that we have treated the quadrature of the single or double layer potential near the singularity, we can obtain similar results for the integral over the doubly periodic surface.

Theorem 3.7. *Let $\alpha \rightarrow x$ be a smooth mapping from \mathbf{R}^2 to \mathbf{R}^3 such that $x(\alpha) - (\alpha, 0)$ is doubly 2π -periodic and (1.13) holds. Let f be a smooth periodic function of α , and G_h^π a regularized periodic Green's function as in (2.1)–(2.3), (2.26). Let $\alpha_j = jh$ for $j \in \mathbf{Z}^2$, and $x_j = x(\alpha_j)$. Then, for each $j \in \mathbf{Z}^2$,*

$$(3.44) \quad \sum_{\ell \in I} G_h^\pi(x_j - x_\ell) f(\alpha_\ell) h^2 - \int G_h^\pi(x_j - x(\alpha')) f(\alpha') d\alpha' = \gamma_j f(\alpha_j) h + O(h^3),$$

where I is the index set (1.10) and the integral is over one period square. Here

$$(3.45) \quad \gamma_j = 2\pi(\det g^{\mu\nu}(\alpha_j))^{1/2} \sum_{0 \neq n \in \mathbb{Z}^2} \Gamma \left(2\pi \sqrt{g^{\mu\nu}(\alpha_j)n_\mu n_\nu} \right),$$

with Γ as in (2.14) and $g^{\mu\nu}$ the inverse metric tensor.

Similarly, let $\tilde{f}(\alpha, \alpha')$ be smooth and periodic in α, α' , and let $n(\alpha')$ be the unit normal vector at $x(\alpha')$. Then the quadrature error for the integral

$$(3.46) \quad \int \nabla G_h^\pi(x_j - x(\alpha')) \cdot n(\alpha') \tilde{f}(\alpha_j, \alpha') d\alpha'.$$

is $O(h)$. If $\tilde{f}(\alpha, \alpha') = 0$ for $\alpha = \alpha'$, the error improves to $O(h^3)$.

Proof. We need to reduce the general case to the local estimates of Lemmas 3.5 and 3.6. As in the proof of Theorem 2.2, we can introduce a cut-off function $\zeta(\alpha)$ with support near zero and write $G_h^\pi(x_j - x(\alpha'))$ as a sum $G_{h0}^\pi(\alpha') + G_{h\infty}^\pi(\alpha')$, depending on j , where the singularity is localized in $G_{h0}^\pi(\alpha')$, and $G_{h\infty}^\pi(\alpha')$ is smooth, with derivatives bounded uniformly in h . We take the domain of integration to be the period square S_j centered at α_j . We can now split the single layer integral into two parts. The integral with $G_{h\infty}^\pi(\alpha')$ has smooth periodic integrand, and its quadrature is high order accurate. The remaining part of the quadrature error comes from the integral with G_{h0}^π . As in the proof of Theorem 2.2, $G_0^\pi(\alpha') = G_h(x_j - x(\alpha'))\zeta(\alpha_j - \alpha')$ for $\alpha' \in S_j$. Thus the single-layer integral is reduced to the case of Lemma 3.5; we need to choose the support of ζ so that (3.25) holds, depending on the mapping $x(\alpha)$. For the double layer integral we use a similar argument to reduce to the case of Lemma 3.6; the hypothesis (3.40) holds when $\tilde{f} = 0$ for $\alpha = \alpha'$. □

We can apply this theorem to the discretization error for the four sums representing integrals in the discrete integral equation (1.25)–(1.27). This error results not only from the quadrature but also from the replacement of the derivative by the discrete operator D_h , and we begin with the latter. If f is a smooth, doubly periodic function of α , we can regard the values of $D_h f$ on the grid as restrictions of a smooth function $D_h f$, defined for all α using the Fourier series for f . Then $D_h f = Df + h^3 r$, where r is a smooth function of α , depending on h , with a high norm bounded uniformly in h . Thus $X_k^{(h)}$, the tangent vector computed using D_h , differs from the exact tangent vector X_k by a smooth function of order h^3 , and similarly for N, n, X_k^* . In the same way, $-D_h^*$ differs from D to $O(h^3)$.

We first compare the integral

$$(3.47) \quad I \equiv \int \nabla^T G_h^\pi(x_j - x(\alpha')) \cdot n(\alpha_j) \phi_n(\alpha') |N(\alpha')| d\alpha'$$

as in (1.26) with the sum

$$(3.48) \quad S \equiv \sum_\ell \nabla_h^T G_h^\pi(x_j - x_\ell) \cdot n_j^{(h)}(\phi_n)_\ell |N_\ell^{(h)}| h^2$$

and derive a correction so that the remaining error is $O(h^3)$. (Upper (h) indicates the use of D_h . We have G_h in the integral since we have already treated the error in regularizing G in §2.) We start by writing out ∇^T in the integral and integrating

by parts to obtain (with sum over $k = 1, 2$ and D_k the derivative in α'_k)

$$(3.49) \quad I = \int G_h^\pi(x_j - x(\alpha')) D_k \{X_k^*(\alpha') \cdot n(\alpha_j) \phi_n(\alpha') |N(\alpha')|\} d\alpha'.$$

Using the remarks above, we can replace $X_k^*(\alpha')$ by $X_k^{*(h)}(\alpha')$ etc., with pointwise error $O(h^3)$. We also replace D_k outside with $-D_{h,k}^*$. Since G_h^π is integrable, the error in the integral is $O(h^3)$. We now have

$$(3.50) \quad I = - \int G_h^\pi(x_j - x(\alpha')) D_{h,k}^* \left\{ X_k^{*(h)}(\alpha') \cdot n_j^{(h)} \phi_n(\alpha') |N^{(h)}(\alpha')| \right\} d\alpha' + O(h^3).$$

Similarly we write out ∇_h^T in the sum and use summation by parts, obtaining

$$(3.51) \quad S = - \sum_\ell G_h^\pi(x_j - x_\ell) D_{h,k}^* \left\{ X_{k\ell}^{*(h)} \cdot n_j^{(h)}(\phi_n)_\ell |N_\ell^{(h)}| \right\} h^2,$$

where $D_{h,k}^*$ acts on the ℓ variable. With the integral and sum in this form, the above theorem applies directly; up to $O(h^3)$, the error is the $O(h)$ term with coefficient $f(\alpha_j)$ given by

$$(3.52) \quad r_j = -D_{h,k}^* \left\{ X_{k\ell}^{*(h)} \cdot n_j^{(h)}(\phi_n)_\ell |N_\ell^{(h)}| \right\} \Big|_{\ell=j}.$$

To simplify this, we can replace $-D_h^*$ by D , use the fact that $X_{kj}^{*(h)} \cdot n_j^{(h)} = 0$, and then replace D with $-D_h^*$, committing $O(h^3)$ errors, to rewrite (3.52) as

$$(3.53) \quad r_j = -(D_{h,k}^* X_k^{*(h)})_j \cdot N_j^{(h)}(\phi_n)_j.$$

In summary, the integral (3.47) and the sum (3.48) differ by

$$(3.54) \quad S - I = \gamma_j r_j h + O(h^3).$$

It is this correction term that appears in (1.26), (1.29) except for the operator P_h . The smoothing by $\rho(k\sqrt{h})$ contributes an error of order $h \cdot h^2 = h^3$, provided $\rho(\xi) - 1 = O(\xi^4)$ as in (1.33).

The first sum in (1.27) can be treated analogously. The correction simplifies since the last factor vanishes at $\ell = j$, and we obtain (1.30). We can use a similar argument to show that the two sums in (1.26), (1.27) with normal derivative of G_h^π differ from the corresponding integrals by $O(h^3)$. After replacing D with D_h again, we have a sum minus an integral with kernel $\nabla G_h^\pi \cdot N_\ell^{(h)}$. We cannot apply the second part of Theorem 3.7 directly, since $N_\ell^{(h)}$ is not exactly normal at $x(\alpha_\ell)$. However, we can write it as the exact $N(\alpha_\ell)$ plus a smooth remainder of order h^3 . The theorem applies to the main part, since the integrand has a factor which vanishes on the diagonal. For the remainder, an argument like Lemmas 3.5 and 3.6 shows that the quadrature for ∇G_h^π has $O(1)$ error, and this is multiplied by $O(h^3)$ in our remainder term. The total quadrature error is thus $O(h^3)$.

4. DISCRETE PSEUDODIFFERENTIAL OPERATORS

In this section we define a class of discrete pseudodifferential operators and derive basic properties such as boundedness on L_h^2 . We use a symbol class which allows us to compose operators by multiplying symbols, in some cases, with bounded remainder. We prove a discrete version of Gårding's inequality and related facts which will be applied to the operator Λ in §6. We interpret discrete integral operators in this

context and express the symbol in terms of the Fourier transform. This connection will be used in §5. For the usual theory of pseudodifferential operators, see e.g., [30]. For an extensive theory of discrete operators with high wavenumber cut-off, see [25].

We will work with operators acting on functions defined on the grid Ih , with I as in (1.10). The general form of a discrete pseudodifferential operator A is

$$(4.1) \quad Af(jh) = (2\pi)^{-2} \sum_{k \in I} \sum_{\ell \in I} a(jh, \ell h, k; h) e^{ik(j-\ell)h} f(\ell h) h^2$$

or

$$(4.1') \quad Af(x) = (2\pi)^{-2} \sum_{k \in I} \sum_{y \in Ih} a(x, y, k; h) e^{ik(x-y)} f(y) h^2, \quad x \in Ih.$$

We generally assume $a(jh, \ell h, k; h)$ is extended periodically to all integer j, ℓ, k . We will often omit the h -dependence in writing a , although it will be important that our estimates have constants independent of h .

In the special case where a is independent of the second variable ℓh or y , we can rewrite the operator (4.1) as

$$(4.2) \quad Af(jh) = \sum_k a(jh, k; h) e^{ikjh} \check{f}(k),$$

where \check{f} is the discrete Fourier transform (1.11). This is the discrete analogue of the standard form of a pseudodifferential operator. On the other hand, if a is independent of the first variable jh or x , we have from (4.1)

$$(4.3) \quad (Af)^\cdot(k) = (2\pi)^{-2} \sum_{\ell} a(\ell h, k; h) e^{-ik\ell h} f(\ell h) h^2.$$

As usual we refer to a as the symbol of the operator A . The following lemma is a direct consequence of the definitions.

Lemma 4.1. *Suppose A is an operator of type (4.2) with symbol $a(jh, k)$ and B is an operator of type (4.3) with symbol $b(\ell h, k)$. Then the composition AB is of type (4.1) with symbol $a(jh, k)b(\ell h, k)$. The adjoint of A is an operator A^* of type (4.3) with symbol $\bar{a}(\ell h, k)$.*

Often we will want to assume that the symbol $a(jh, \ell h, k; h)$ is smooth in $jh, \ell h$ with order m in k , at least in the sense that

$$(4.4) \quad |D_+^s a(jh, \ell h, k; h)| \leq C(|k| + 1)^m$$

with C independent of $jh, \ell h \in Ih, k \in I$, as well as h . Here s is a multi-index, arbitrary up to some large order, and D_+ is a forward divided difference in jh or ℓh . The next lemma gives the L_h^2 boundedness of an operator with such a symbol with order $m = 0$.

Lemma 4.2. *Assume (4.4) holds with $m = 0$ and with s large. Then*

(i) *The discrete transform $\check{a}(\xi, \eta, k; h)$ of a with respect to (x, y) satisfies*

$$(4.5) \quad |\check{a}(\xi, \eta, k; h)| \leq C(1 + |\xi|^2 + |\eta|^2)^{-\nu/2}$$

with ν large depending on s .

(ii) *The operator A defined by (4.1) is bounded in norm on L_h^2 uniformly in h .*

Proof. For (i), we note that the five-point Laplacian of a in jh is bounded by hypothesis, and therefore its transform $-4h^{-2}(\sin^2(\xi_1 h/2) + \sin^2(\xi_2 h/2))\ddot{a}(\xi, \eta, k)$ is also. This is at least $(2/\pi)^2|\xi|^2|\ddot{a}|$ in magnitude. Similarly, using powers of the discrete Laplacian in jh or ℓh , we obtain the estimate (4.5).

Part (ii) can be proved by adapting a standard argument, e.g., [30], Prop. II.6.1. With $x, y \in Ih$ we can write

$$(4.6) \quad a(x, y, k) = \sum_{\xi, \eta \in I} \ddot{a}(\xi, \eta, k)e^{i\xi x}e^{i\eta y}, \quad A = \sum_{\xi, \eta \in I} A_{\xi\eta},$$

$$(4.7) \quad A_{\xi\eta}f(x) = (2\pi)^{-2} \sum_k \sum_\ell \ddot{a}(\xi, \eta, k)e^{i\xi x}e^{i\eta \ell h}e^{ik(x-\ell h)}f(\ell h)h^2.$$

Now

$$(4.8) \quad A_{\xi\eta}f(x) = \sum_{k \in I} e^{i(k+\xi)x}\ddot{a}(\xi, \eta, k)\ddot{f}(k-\eta).$$

Each factor is periodic in k , and we can shift k to rewrite this as

$$(4.9) \quad A_{\xi\eta}f(x) = \sum_{k \in I} e^{i(k+\xi+\eta)x}\ddot{a}(\xi, \eta, k+\eta)\ddot{f}(k).$$

Thus $A_{\xi\eta}f(x)$ is $e^{i(\xi+\eta)x}$ times a function whose transform is $\ddot{a}(\xi, \eta, k+\eta)\ddot{f}(k)$. It follows from (i) that $|A_{\xi\eta}f|_{L^2} \leq C((1+|\xi|^2+|\eta|^2)^{-\nu/2}|f|_{L^2})$. Then $|Af|_{L^2}$ is bounded by the sum of such estimates; we obtain the result provided ν is large enough so that the sum over ξ, η has an upper bound independent of h . \square

For further results we need an assumption that the undivided difference in k , written as $\Delta_{+(k)}$, reduces the order of the symbol by 1. For this reason we define a symbol class somewhat like that of the continuous case. We will say that $a(x, y, k; h)$ is a **symbol of class S^m** , for real m , if $a(x, y, k; h)$ is defined for all $x, y \in R^2$ and integer k , is periodic in each variable, and satisfies the estimate

$$(4.10) \quad |\Delta_{+(k)}^n D^s a(x, k; h)| \leq C(1+|k|)^{m-|n|}, \quad k \in I, \quad |n| = 0 \text{ or } 1,$$

where n and s are multi-indices and D^s is an (x, y) -derivative, with s up to large degree. Note that (4.10) is required to hold even at the border points of I . We are primarily interested in the special case of a symbol for an operator of type (4.2) or (4.3). The following lemma shows that the composition of two operators of type (4.2) and (4.3) with total order ≤ 1 can be written as an operator of type (4.2) plus a bounded remainder.

Lemma 4.3. *Let $a(x, k; h)$, $b(y, k; h)$ be symbols of class S^{m_1} , S^{m_2} , $m_1 + m_2 \leq 1$. Let A, B be the operators of type (4.2), (4.3) corresponding to $a(jh, k; h)$, $b(\ell h, k; h)$. Also let M be the operator of type (4.2) with symbol $a(jh, k; h)b(jh, k; h)$. Then $M - AB$ is bounded as an operator on L_h^2 , uniformly in h .*

Proof. The operator $M - AB$ has type (4.1) with symbol $a(x, k)(b(x, k) - b(y, k))$. We want to perform a summation by parts using

$$(4.11) \quad \Delta_{+\nu} e^{ik(x-y)} = \left(e^{i(x_\nu - y_\nu)} - 1 \right) e^{ik(x-y)},$$

where $\Delta_{+\nu}$ is the forward difference in k_ν . We can write

$$(4.12) \quad b(x, k) - b(y, k) = \sum_{\nu=1,2} q_\nu(x, y, k) \left(e^{i(x_\nu - y_\nu)} - 1 \right)$$

with

$$(4.13) \quad q_1 = \frac{b(x_1, x_2, k) - b(y_1, x_2, k)}{e^{i(x_1 - y_1)} - 1}, \quad q_2 = \frac{b(y_1, x_2, k) - b(y_1, y_2, k)}{e^{i(x_2 - y_2)} - 1}.$$

The denominator in q_ν vanishes only where $x_\nu = y_\nu$ modulo 2π , and q_ν can be extended there so that q_ν is smooth and periodic in x, y . It can be checked that q_ν satisfies the same estimates as b . We now have

$$(4.14) \quad (M - AB)f(x) = (2\pi)^{-2} \sum_{\nu, k, y} a(x, k)q_\nu(x, y, k)\Delta_{+\nu}e^{ik(x-y)}f(y)h^2,$$

or, with a summation by parts,

$$(4.15) \quad (M - AB)f(x) = -(2\pi)^{-2} \sum_{\nu, k, y} \Delta_{-\nu}(a(x, k)q_\nu(x, y, k))e^{ik(x-y)}f(y)h^2,$$

using the periodicity in k . The estimates for a, b, q_ν imply that $\Delta_{-\nu}D_{x,y}^s(aq_\nu)$ is uniformly bounded for large s , independent of k, h , and the same holds if the (x, y) -derivatives are replaced by differences. Finally we can conclude from Lemma 4.2 that the operator $M - AB$ is L_h^2 -bounded, independent of h . \square

The next three results use this lemma. It is convenient to use an operator E on grid functions representing an absolute first derivative, defined as

$$(4.16) \quad (Ef)''(k) = (1 + |k|^2)^{1/2}\ddot{f}(k), \quad k \in I.$$

More generally, we define E^r as multiplication by $(1 + |k|^2)^{r/2}$ in the transform for real r . It is important to us that this factor is itself in class S^r , i.e., first differences in k of the periodic extension reduce the order in k .

Lemma 4.4. *Let A be an operator of type (4.2) with symbol $a(x, k; h)$ in the class S^1 . Then there are operators B_1, B_2, B_3 , bounded on L_h^2 uniformly in h , so that*

$$(4.17) \quad A = B_1E, \quad A = EB_2, \quad A = E^{1/2}B_3E^{1/2}.$$

Proof. Let $b(x, k; h) = a(x, k; h)\eta(k)^{-1}$ for $k \in I$, where $\eta(k) = (1 + |k|^2)^{1/2}$, and extend periodically in k . Then b is a symbol of class S^0 . Let B_1 be the operator of type (4.2) with symbol $b(x, k; h)$. Then B_1 is bounded uniformly in h , according to Lemma 4.2, and $A = B_1E$. This gives the first equation. For the second, we start with $B_0 \equiv B_1^*$, a bounded operator of type (4.3) with symbol $b(y, k; h)$. We apply Lemma 4.3 with E, B_0 in place of A, B , and $m_1 = 1, m_2 = 0$. We conclude that EB_0 differs by a bounded operator from the type (4.2) operator with symbol $\eta(k)b(x, k; h)$, namely A . Thus we have $A = EB_0 + B_2$ for some B_2 , or $A = E(B_0 + E^{-1}B_2)$, which is the second equation except for notation.

The third equation is proved similarly. Let R be the operator of type (4.2) with symbol $r(x, k; h) = a(x, k; h)\eta(k)^{-1/2}$ for $k \in I$, so that r is of class $S^{1/2}$, $A = RE^{1/2}$, and $r = \eta(k)^{1/2}b$. We apply Lemma 4.3 to the operators $E^{1/2}, B_0$, with B_0 as above, and conclude that $R = E^{1/2}B_0 + B_4$ for some bounded B_4 . Then $A = (E^{1/2}B_0 + B_4)E^{1/2} = E^{1/2}(B_0 + E^{-1/2}B_4)E^{1/2}$. \square

Next we derive a result like Gårding's inequality, relating the positivity of a symbol of class S^1 to the positivity of the operator. The resulting estimate is crucial for the numerical stability estimates of §6.

Lemma 4.5. *Let $a(x, k; h)$ be a symbol of class S^1 . Assume that $a(x, k; h) \geq c_0|k|$ for $k \in I$ and all x , with constant $c_0 > 0$. Let A be the operator of type (4.2) with symbol $a(x, k; h)$. Then $A^* - A$ is L_h^2 -bounded, uniformly in h , and for all grid functions f and some $C \geq 0$,*

$$(4.18) \quad \operatorname{Re}(Af, f)_{L_h^2} \geq \frac{c_0}{2} \sum_{k \in I} |k| |\dot{f}(k)|^2 - C|f|_{L_h^2}^2.$$

Proof. We mimic the standard proof (e.g., [30], Lemma II.6.2), using Lemma 4.3. We may assume that $a(x, k; h) \geq c_0\eta(k)$ for $k \in I$, where $\eta(k) = (1 + |k|^2)^{1/2}$, by adding a constant to a without affecting the conclusion. We set $b(x, k; h) = a(x, k; h)/\eta(k)$ for $k \in I$ and extend periodically in k . Then b is a symbol of class S^0 . Let $a_1(x, k; h) = a(x, k; h) - (c_0/2)\eta(k)$ for $k \in I$, and let $A = A_0 + A_1$, where A_0 has symbol $(c_0/2)\eta(k)$ and A_1 has symbol $a_1(x, k; h)$, $k \in I$. Then $a_1(x, k; h) = \eta(k)(b(x, k; h) - c_0/2)$ for $k \in I$; note the last factor is at least $c_0/2$. We want to approximate A_1 by an operator of the form RR^* , which is necessarily positive. Let $r(x, k) = \eta(k)^{1/2} [b(x, k; h) - c_0/2]^{1/2}$. We check that r is a symbol of class $S^{1/2}$: The bound for $D_x^s r$ follows from the one for $D_x^s b$. As for the k -difference, the estimate for $\Delta_{+(k)} D_x^s b$ implies that $|\Delta_{+(k)} D_x^s [b(x, k; h) - c_0/2]^{1/2}| \leq C\eta(k)^{-1}$ and therefore $|\Delta_{+(k)} D_x^s r(x, k; h)| \leq C\eta(k)^{-1/2}$. Thus Lemma 4.3 applies to the operator R with symbol $r(x, k; h)$ and the adjoint R^* with symbol $r(y, k; h)$. We conclude that $A_1 = RR^* + B$ with B bounded. Since RR^* and A_0 are self-adjoint, $A^* - A = B^* - B$, and the first statement is proved. Further, we have

$$(4.19) \quad (Af, f)_{L_h^2} = (A_0f, f)_{L_h^2} + |R^*f|_{L_h^2}^2 + (Bf, f)_{L_h^2},$$

and the second statement follows. □

The next lemma expresses the absolute derivative E in terms of the operator A of Lemma 4.5; this is needed in §6.

Lemma 4.6. *Let A be as in Lemma 4.5. Then for each h there are operators B_4, B_5 , bounded on L_h^2 uniformly in h , so that $E = B_4A + B_5$.*

Proof. Let Q be the operator of type (4.3) with symbol b^{-1} , where $b = a/\eta$ for $k \in I$. Lemma 4.3 applies with A, Q in place of A, B , and $m_1 = 1, m_2 = 0$. We conclude that AQ differs by a bounded operator from the operator of type (4.2) with symbol $ab^{-1} = \eta$; That is, $AQ = E + B_1$ for some bounded B_1 . Now Q is bounded, according to Lemma 4.2. Taking adjoints, we get $Q^*A^* = E + B_1^*$. Then, since $A^* - A \equiv B_3$ is a bounded operator, we have $B_4A = E + B_1^* - B_4B_3$, with $B_4 = Q^*$, or $E = B_4A + B_5$. □

In dealing with discrete potentials, we will apply the above to discrete integral operators of the form

$$(4.20) \quad Af(jh) = \sum_{\ell \in I} K^\pi(jh, jh - \ell h) f(\ell h) h^2,$$

where $K^\pi(x, z)$ is periodic in both x and z , and K^π has the form

$$(4.21) \quad K^\pi(x, z) = \sum_{n \in \mathbb{Z}^2} K(x, z + 2\pi n)$$

for a function $K(x, z)$ which is smooth in x and z , periodic in x , and rapidly decreasing in z . For each j , we can regard the sum (4.20) as a discrete convolution

of $K^\pi(jh, \cdot)$ with f , evaluated at jh . Then Af is the inverse discrete transform of a product,

$$(4.22) \quad Af(jh) = (2\pi)^2 \sum_{k \in I} \ddot{K}^\pi(jh, k) e^{ikjh} \dot{f}(k),$$

an operator of type (4.2). Furthermore, since K^π has the form (4.21), its transform as a discrete periodic function can be written as a discrete transform of K itself,

$$(4.23) \quad \ddot{K}^\pi(jh, k) = (2\pi)^{-2} \sum_{m \in \mathbb{Z}^2} K(jh, mh) e^{-ikmh} h^2.$$

The latter can be related to the usual Fourier transform of K , as a function of z , using the Poisson summation formula (3.1):

$$(4.24) \quad \ddot{K}^\pi(jh, k) = (2\pi)^{-1} \sum_{n \in \mathbb{Z}^2} \hat{K}(jh, k + 2\pi n/h).$$

This relation will allow us to study operators related to G_h^π by estimating their transforms, and to derive an important positivity property using Lemma 4.5.

5. ESTIMATES FOR INTEGRAL OPERATORS

In this section we derive boundedness properties on L_h^2 of discrete integral operators with kernels related to the regularized Green’s function. We expand G_h near the singularity into terms where derivatives of G_h are composed with the linearized coordinate mapping. The Fourier transforms of such terms are estimated. It is then shown, using the results of §4, that various operators are bounded, with gain of derivatives as for the original integrals.

We consider operators of the form

$$(5.1) \quad Af(\alpha_j) = \sum_{\ell \in I} K(\alpha_j, \alpha_\ell) f(\alpha_\ell) h^2$$

acting on grid functions f . The kernel K will be related to

$$G_h^\pi(x_j - x_\ell) = G_h^\pi(x(\alpha_j) - x(\alpha_\ell)).$$

In order to say that certain operators gain derivatives in L_h^2 , we use the operator E defined in (4.16), representing an absolute derivative in a discrete sense. Thus if A is an operator of type (4.2) such that $|a(x, k; h)| \leq C(1 + |k|^2)^{-n/2}$ for some $n \geq 0$, with the same estimate for x -derivatives of a , then AE^n is bounded on L_h^2 , uniformly in h , according to Lemma 4.2, i.e., A gains n derivatives. When AE^n is bounded in this sense for $n \geq 0$, we will say that A is of order $-n$ as an operator on L_h^2 . The following theorem summarizes properties of discrete operators associated with G_h which will be needed for the stability estimates for the scheme.

Theorem 5.1. *Suppose that the regularized Green’s function G_h satisfies the assumptions (2.1)–(2.3) and $\hat{G}_h(k) < 0$. Let A be the operator*

$$(5.2) \quad Af(\alpha_j) = \sum_{\ell \in I} G_h^\pi(x_j - x_\ell) f(\alpha_\ell) h^2.$$

Then A is of order -1 , i.e., AE is bounded on L_h^2 uniformly in h . Specifically, A has the form $A = -A^{(1)} - A^{(2)}$, where $A^{(1)}$ has order -1 , $A^{(2)}$ has order -2 , and

$A^{(1)}$ is an operator of type (4.2) whose symbol $a_1(\alpha, k; h)$ is of class S^{-1} , in the sense of (4.10), and also satisfies, for some $c_1 > 0$,

$$(5.3) \quad a_1(\alpha, k; h) \geq c_1(1 + |k|^2)^{-1/2}.$$

More generally, suppose \tilde{x}_j approximates $x_j = x(\alpha_j)$, with $|\tilde{x}_j - x_j| \leq c_0h$ for each j , and $\tilde{x}_j - x_j$ is periodic. Let $\mu(\alpha, \alpha')$ be an arbitrary smooth, periodic function, and let A_m be the operator of the form (5.1) which has the kernel $\mu(\alpha_j, \alpha_\ell)D_x^m G_h^\pi(\tilde{x}_j - \tilde{x}_\ell)$, where D_x^m is a derivative of order $|m|$ for multi-index m . Then A_m is of order -1 for $m = 0$ and order 0 for $|m| = 1$. For $|m| = 2$, the operator hA_m is of order 0 . In the special case that $\mu = 0$ on the diagonal $\alpha = \alpha'$, the operator A_m has order $|m| - 2$ for $0 \leq |m| \leq 2$. Also for arbitrary μ the operator with kernel $\mu \partial G_h^\pi(x_j - x_\ell) / \partial n$ is of order -1 , where n denotes either normal vector $n(x_j)$ or $n(x_\ell)$.

We also need a more special result concerning the discrete derivative of G_h , showing an extra gain of a derivative due to a smooth factor μ which vanishes on the diagonal.

Theorem 5.2. *With G_h as above, let D_h be a first order derivative operator as in (1.14)–(1.16), and let $\mu(\alpha, \alpha')$ be smooth and periodic, with $\mu = 0$ when $\alpha = \alpha'$. Then the following two operators are bounded on L_h^2 uniformly in h , where both D_h and E act with respect to α_ℓ :*

$$(5.4) \quad B_1 f(\alpha_j) = \sum_{\ell \in I} D_h G_h^\pi(x_j - x_\ell) \mu(\alpha_j, \alpha_\ell) E f(\alpha_\ell) h^2,$$

$$(5.5) \quad B_2 f(\alpha_j) = \sum_{\ell \in I} E^2 G_h^\pi(x_j - x_\ell) \mu(\alpha_j, \alpha_\ell) f(\alpha_\ell) h^2$$

To begin deriving these facts, we first split the Green’s function into a far-field part and a local part, in order to focus attention on the latter. We wish to restrict the local analysis to a small neighborhood of the singularity in which the coordinate mapping is well approximated by its linearization. Let $J(\alpha)$ be the Jacobian matrix $\partial x / \partial \alpha$ at α . Because of (1.13) and the smoothness of $x(\alpha)$, there is some δ_0 small enough so that $\delta_0 < \pi/2$ and

$$(5.6) \quad |J(\alpha)(\alpha - \alpha')|/2 \leq |x(\alpha) - x(\alpha')| \leq 2|J(\alpha)(\alpha - \alpha')|, \quad |\alpha - \alpha'| \leq \delta_0.$$

Also from (1.13) there exists $r_0 > 0$ with $r_0 < \pi/2$ so that $|x(\alpha) - x(\alpha')| \leq r_0$ implies $|\alpha - \alpha'| \leq \delta_0$. We can also assume that $|J(\alpha)(\alpha - \alpha')| \leq r_0$ implies $|\alpha - \alpha'| \leq \delta_0$. We now choose a cut-off function $\zeta : \mathbf{R}^3 \rightarrow \mathbf{R}$ so that $\zeta(x) = 1$ for x near 0 and $\zeta(x) = 0$ for $|x| > r_0$. Thus (5.6) holds whenever $x(\alpha) - x(\alpha')$ is within the support of ζ . We write the regularized Green’s function as $G_h = \zeta G_h + (1 - \zeta)G_h$. The periodic version is then split as $G_h^\pi = G_{h0}^\pi + G_{h\infty}^\pi$, as in Theorem 2.2. The far-field part $G_{h\infty}^\pi$ is smooth and periodic. Consequently a discrete integral operator with kernel $D^m G_{h\infty}^\pi(x_j - x_\ell)$ is L_h^2 -bounded, uniformly in h , for D^m an x -derivative of any order m . The local term G_{h0}^π when evaluated on the surface is

$$(5.7) \quad G_{h0}^\pi(x(\alpha) - x(\alpha')) = G_h(x(\alpha) - x(\alpha')) \zeta(x(\alpha) - x(\alpha'))$$

when $|\alpha'_\nu - \alpha_\nu| \leq \pi$; the remaining terms in the sum are zero because of the small support of ζ . Thus the boundedness properties of a discrete operator with kernel $D^m G_h^\pi(x_j - x_\ell)$ reduce to consideration of $D^m(G_{h0})(x_j - x_\ell)$, where $G_{h0}(x) = G_h(x)\zeta(x)$.

We now consider the boundedness properties of the operator (5.2). Because of the above remarks, we replace G_h^π by G_{h0}^π . We will make a Taylor expansion of the kernel, which will enable us to use the representation (4.20) for the resulting terms. We treat $x_j - x_\ell$ as a perturbation of its linearization $y_{j\ell} = J_j(\alpha_j - \alpha_\ell)$, where $J_j = J(\alpha_j)$. Thus we can write $G_{h0}^\pi(x_j - x_\ell)$ as an expansion in terms $D_x^m G_{h0}^\pi(y_{j\ell})(z_{j\ell})^m$, summed over m with remainder, where $z_{j\ell} = x(\alpha_j) - x(\alpha_\ell) - y_{j\ell}$, and m is a multi-index. We can further expand $z_{j\ell}$ in powers of $\alpha_j - \alpha_\ell$, quadratic or higher. We then have a linear combination of terms, a typical one being, for $|\alpha_{\ell\nu} - \alpha_{j\nu}| < \pi$,

$$(5.8) \quad D_x^m G_{h0}^\pi(y_{j\ell})(\alpha_j - \alpha_\ell)^p = D_x^m G_{h0}^\pi(J_j(\alpha_j - \alpha_\ell))(\alpha_j - \alpha_\ell)^p.$$

Here p is another multi-index, with $|p| \geq 2|m|$. The discrete integral operator with (5.8) as kernel, extended periodically, has the form (4.20), and therefore (4.22), with symbol given by (4.24). Thus we can derive boundedness properties of this operator by estimating the Fourier transform of the kernel $\alpha^p D_x^m G_{h0}^\pi(J_j \alpha)$ with respect to α . The relevant estimates are stated in the following lemma. The rapid decay for kh large is needed for the convergence of the sum (4.24). These estimates and the previous remarks show that the operator with kernel (5.8) gains $|p| + 1 - |m|$ derivatives, i.e., it is of order $|m| - |p| - 1$ on L_h^2 in the sense defined above.

Lemma 5.3. *Let $K_{mp}(\alpha) = \alpha^p D_x^m G_{h0}^\pi(J\alpha)$, where J is the Jacobian matrix at some fixed α_0 . Assume that $|p| + 1 \geq |m|$. Then the Fourier transform \hat{K}_{mp} satisfies the following estimates uniformly in h :*

$$(5.9) \quad |\hat{K}_{mp}(k)| \leq \begin{cases} C, & |k| \leq 1, \\ C|k|^{|m|-|p|-1}, & 1 \leq |k| \leq C_0/h, \\ Ch^{-|m|+|p|+1}|kh|^{-n}, & |k| \geq 1/h, \end{cases}$$

with n large. Similar estimates hold for the derivatives of \hat{K}_{mp} with respect to α_0 . The same estimates hold for $|k| \geq 1$ if G_{h0} is replaced by G_h . For $p = 0$ and $|m| = 2$, we have the same estimate for $|k| > 1/h$, and $|\hat{K}_{mp}(k)| \leq Ch^{-1}$ for $|k| \leq C_0/h$.

In the rest of this section we present the proof of the Lemma 5.3, then the proofs of Theorems 5.1 and 5.2, and one final lemma.

Proof of Lemma 5.3. In estimating this transform it is helpful to note that the x -derivatives on G_h can be replaced by α -derivatives, as we now explain. First we extend the Jacobian $J : \mathbf{R}^2 \rightarrow \mathbf{R}^3$ at α_0 to a nonsingular operator $\tilde{J} : \mathbf{R}^3 \rightarrow \mathbf{R}^3$ by defining

$$(5.10) \quad \tilde{J}(\alpha_1, \alpha_2, \alpha_3) = J(\alpha_1, \alpha_2) + \alpha_3 N,$$

where $N = X_1 \times X_2$ and X_1, X_2 are the tangent vectors at α_j , as before. Now since G_h is radial, $(\nabla G_h)(J\alpha)$ has the direction of $J\alpha$ for $\alpha \in R^2$, and thus is perpendicular to N , so that $(\nabla G_h)(J\alpha) = (G_h \circ J)_{\alpha_1} X_1^* + (G_h \circ J)_{\alpha_2} X_2^*$. Thus $D_x G_h$ can be replaced with $D_\alpha(G_h \circ J)$. Next we note that the matrices of second derivatives are related by $D_\alpha^2(G_h \circ \tilde{J}) = \tilde{J}^*(D_x^2 G_h)\tilde{J}$. This shows that $D_x^2 G_h$ can be expressed in α -derivatives of $G_h \circ \tilde{J}$ for $\alpha \in R^3$. However, for $\alpha_3 = 0$ we have $\partial(G_h \circ \tilde{J})/\partial\alpha_3 = 0$, and the same is true for the second partials in α_3, α_1 or α_3, α_2 . Also the second partial in α_3, α_3 can be rewritten in α_1, α_2 -derivatives plus a multiple of $\psi_h \circ \tilde{J}$, since $\Delta G_h = \psi_h$. Thus we have reduced the second

x -derivatives to α_1, α_2 -derivatives plus the ψ_h term. For higher derivatives, we can convert $D_x^m G_h(\tilde{J}\alpha)$ to $D_\alpha^m(G_h \circ \tilde{J})$ for $\alpha \in \mathbf{R}^3$, and then repeat the above process, converting to α_1, α_2 -derivatives, until a term with ψ_h appears. In summary, a term of the form $D_x^m G_h(J\alpha)$ with $\alpha \in R^2$ can be replaced by a sum of terms of the form $D_\alpha^m(G_h \circ J)$, with α_1, α_2 -derivatives only, and $D_x^{m-2}\psi_h(J\alpha)$.

We first estimate the transform of $F_{mp}(\alpha) = \alpha^p D_\alpha^m(G_h(J\alpha))$. (We ignore the cut-off ζ for now and account for its effect later.) First, since $\Delta G_h = \psi_h$, we have $\hat{G}_h(k) = -\hat{\psi}_h(k)/|k|^2 = -\hat{\psi}(kh)/|k|^2$ for the 3-D transforms. Now, as in §2, we obtain the two-dimensional transform of $G_h \circ J$ from

$$(5.11) \quad (G_h \circ J)^\wedge(k) = C \int_{-\infty}^{\infty} \hat{G}_h(M(k, \ell)) \, d\ell = C \int_{-\infty}^{\infty} |M(k, \ell)|^{-2} \hat{\psi}(M(k, \ell)h) \, d\ell,$$

where $k \in \mathbf{R}^2$ and $M = (\tilde{J}^*)^{-1}$, with \tilde{J} as above. To obtain the transform of $\alpha^p D_\alpha^m(G_h(J\alpha))$, we need to multiply this by $(ik)^m$ and then apply $(i\partial_k)^p$. We obtain various terms where e.g., q derivatives apply to $\hat{\psi}$ and the remaining $|p| - q$ apply to $k^m |M(k, \ell)|^{-2}$. It is important that $|M(k, \ell)|^2$ depends on ℓ only through an ℓ^2 term; this follows from the definition of \tilde{J} . Thus $\partial_k |M(k, \ell)|^2$ is linear in k , without ℓ dependence. The resulting term has the form

$$(5.12) \quad C \int_{-\infty}^{\infty} k^s h^q |M(k, \ell)|^{-n} (\partial^q \hat{\psi})(M(k, \ell)h) \, d\ell$$

with $n \geq 2$, and the total degree in k has been lowered by $|p| - q$, i.e., $s - n = |m| - 2 - |p| + q$. If we let $\kappa = |kh|$ and $\xi = \ell h$, and convert the integral to ξ , we see that the integral is dominated by

$$(5.13) \quad C |k|^s h^{q+n-1} \int_{-\infty}^{\infty} (\kappa^2 + \xi^2)^{-n/2} (1 + \kappa^2 + \xi^2)^{-N/2} \, d\xi$$

for some large N ; we have used the smoothness of ψ . We first estimate this assuming $k \neq 0$ and $|kh| \leq C_0$. In this case we drop the last factor in the integral (the resulting integral exists since $n \geq 2$) and convert the integral to ξ/κ . We find that the integral is of order κ^{-n+1} , and consequently the entire term above is bounded by $C |k|^s h^{q+n-1} \kappa^{-n+1} = |k|^{|m|-|p|-1} (|kh|^q)$, and in summary

$$(5.14) \quad |\hat{F}_{mp}(k)| \leq C |k|^{|m|-|p|-1}, \quad |kh| \leq C_0, \quad k \neq 0.$$

On the other hand, for $|kh| \geq 1$, we return to (5.13), drop the 1 in the second factor, and find that the integral is of order $|\kappa|^{-(n+N-1)}$. The expression (5.13) is then bounded by $C |\kappa|^{s-(n+N-1)} h^{q+n-1-s} = C |\kappa|^{s-(n+N-1)} h^{-|m|+|p|+1}$. The power of $\kappa = |kh|$ can be made large negative by taking N large, and we obtain

$$(5.15) \quad |\hat{F}_{mp}(k)| \leq C h^{-|m|+|p|+1} |kh|^{-n}, \quad |kh| \geq 1.$$

We need a similar estimate for the transform of $P_{mp}(\alpha) = \alpha^p (D_x^{m-2}\psi_h)(J\alpha)$. Omitting the α^p factor for the moment, we have

$$(5.16) \quad ((D_x^{m-2}\psi_h) \circ J)^\wedge(k) = C \int_{-\infty}^{\infty} |M(k, \ell)|^{m-2} \hat{\psi}(M(k, \ell)h) \, d\ell.$$

To obtain the transform of P_{mp} , we apply ∂_k^p to the above. If q derivatives apply to the $\hat{\psi}$ factor and $|p| - q$ apply to the first factor, we obtain an expression

$$(5.17) \quad \int_{-\infty}^{\infty} \Phi(k, \ell) h^q (\partial^q \hat{\psi})(M(k, \ell)h) d\ell,$$

where Φ is homogeneous of degree $s = |m| - 2 - |p| + q$. We now rewrite this with $\kappa = |kh|$, $\xi = \ell h$ and estimate by

$$(5.18) \quad h^{q-s-1} \int_{-\infty}^{\infty} (\kappa^2 + \xi^2)^{s/2} (1 + \kappa^2 + \xi^2)^{-N/2} d\xi$$

for large N . For $k \neq 0$ and $\kappa = |kh| \leq C_0$ we replace the integrand in (5.18) by $(1 + \kappa^2 + \xi^2)^{-(N-s)/2}$. The integral is $O(1)$, and the term is of order $h^{q-s-1} = h^{-|m|+|p|+1}$; that is,

$$(5.19) \quad |\hat{P}_{mp}(k)| \leq Ch^{-|m|+|p|+1}, \quad |kh| \leq C_0, \quad k \neq 0.$$

If the exponent of h is ≥ 0 , we can majorize by $C|k|^{|m|-|p|-1}$, as in the estimate (5.14) for \hat{F}_{mp} . On the other hand, for $|kh| \geq 1$, we drop the 1 in the second factor in (5.18), and find that the integral is of order κ^{-n} for large n , so that

$$(5.20) \quad |\hat{P}_{mp}(k)| \leq Ch^{-|m|+|p|+1}|kh|^{-n}, \quad |kh| \geq 1.$$

Next we consider the cut-off function ζ . We first show that the difference in the transform due to ζ is negligible for $|k| \geq 1$, i.e., we show that the transform of

$$(5.21) \quad Q_{mp}(\alpha) = \alpha^p D_x^m G_h(J\alpha) \cdot (1 - \zeta(J\alpha))$$

is rapidly decreasing for large k . If we apply D_α^s to Q_{mp} with s of large degree, we can estimate using the chain rule and the fact that $|D_x^\ell G_h(x)| \leq C|x|^{-\ell-1}$ for $|x| \geq h$. We find that $|D_\alpha^s Q_{mp}(\alpha)| \leq C|\alpha|^{|p|-|m|-1-|s|}$, and of course $Q_{mp}(\alpha) = 0$ for α near 0 and for α large. Thus $D_\alpha^s Q_{mp}$ is bounded in L^1 independent of h for $|s|$ large. This implies that $|\hat{Q}_{mp}(k)| \leq C|k|^{-N}$ for $|k| \geq 1$ with N large. This estimate is small enough that it will not affect the estimates already obtained for $|k| \geq 1$ when F_{mp} , P_{mp} are multiplied by $\zeta(J\alpha)$. There are additional terms where ζ is differentiated, but these terms vanish near 0; consequently their derivatives are bounded independent of h , and the transform is again rapidly decreasing.

It remains to estimate the transforms of $F_{mp}(\alpha)\zeta(J\alpha)$ and $P_{mp}(\alpha)\zeta(J\alpha)$ for $|k| \leq 1$. In the first case the transform is

$$(5.22) \quad (2\pi)^{-1} \int \alpha^p D_\alpha^m (G_h(J\alpha)) e^{-ik\alpha} \zeta(J\alpha) d^2\alpha.$$

We can integrate by parts so that the m derivatives apply to $\alpha^p e^{-ik\alpha} \zeta(J\alpha)$. The result is an integrand bounded by $|G_h(J\alpha)|$, for $|k| \leq 1$, over the support of ζ . Since $|G_h(x)| \leq h^{-1}$ and $|G_h(x)| \leq |x|^{-1}$ for $|x| \geq h$, we can easily show that this last integral is independent of h . For the case of $P_{mp}\zeta$ we cannot integrate by parts because we have x -derivatives; however, we can use the scaling of ψ_h in h to show that the transform is bounded by $Ch^{-|m|+|p|+1}$.

Finally, combining the estimates (5.14), (5.15), (5.19), (5.20) and the last two paragraphs, we obtain the estimates stated for \hat{K}_{mp} . It can be checked that derivatives in α_0 do not seriously affect the estimates, so that the same bounds can be obtained in this case; the dependence on α_0 is through $J = J(\alpha_0)$ in K_{mp} and therefore through M in the transform. \square

Proof of Theorem 5.1. We first consider the operator (5.2). As explained before, we reduce consideration to G_{h0}^π and form the Taylor expansion in terms (5.8). The operator with kernel (5.8) has the form (4.20), (4.22), with symbol given by (4.24), and it follows from the estimates of Lemma 5.3 and from Lemma 4.2 that this operator is bounded of order $|m| - |p| - 1$. The first term, with $m = p = 0$, is of order -1 and the others -2 or less, since $|p| \geq 2|m|$. It remains to show that the remainder is of order -2 . Suppose we carry the expansion for G_{h0}^π to terms with $|m| < N$ and the one for $z_{j\ell}$ to terms of degree $\leq N$ in α . Then we have two kinds of remainders: One has the form $F_N(\alpha_j, \alpha_\ell)(z_{j\ell})^N$, where F_N is an average of $D_x^N G_{h0}^\pi$ over the line from $y_{j\ell}$ to $x_j - x_\ell$. The other type of remainder, from expanding $z_{j\ell}$, is $D_x^m G_{h0}^\pi(y_{j\ell})(\alpha_j - \alpha_\ell)^p g(\alpha_j - \alpha_\ell)$, where g is some smooth function and $|p| \geq N + 2|m| - 1$. It is routine to check that derivatives up to order $N - 1$ of either remainder with respect to α_ℓ , treated as a continuous variable, are uniformly bounded. We can use this fact to estimate the remainders crudely. We need to show that RE^2 is bounded as an operator on L^2 , where R is the operator corresponding to a remainder term. If R has kernel $R(\alpha_j, \alpha_\ell)$, we can regard $(RE^2 f)(\alpha_j)$ as the inner product of $R(\alpha_j, \cdot)$ with $E^2 f$. Since E^2 is self-adjoint, this will be uniformly bounded by $|f|_{L^2}$ provided $E^2 R(\alpha_j, \cdot)$ is bounded uniformly in α_j, α_ℓ , where E^2 acts on the α_ℓ variable. It can be shown that the spectral derivative $E^2 R$ is bounded by derivatives $D_\alpha^m R$ for $|m| \leq 5$ (cf. [31], pp. 250-4), and thus the operator RE^2 is bounded provided $N \geq 6$.

The decomposition $A = -A^{(1)} - A^{(2)}$ essentially follows from separating out the leading term in the expansion, namely $G_{h0}^\pi(J(\alpha_j)(\alpha_j - \alpha_\ell))$. This term contributes to A an operator of the form (4.22) whose symbol is given by (4.24) with K replaced by $G_{h0} \circ J$. Since $\hat{G}_h(k) < 0$, and since $(G_{h0} \circ J)^\wedge(k) - (G_h \circ J)^\wedge(k)$ decreases rapidly for large k , as seen below (5.21), we will take $A^{(1)}$ to be a similar operator with kernel K whose transform agrees with $(-G_h \circ J)^\wedge(k)$ for large k . Let $\chi : [0, \infty) \rightarrow [0, 1]$ be a smooth function with $\chi(r) = 1$ for $r \leq 1$ and $\chi(r) = 0$ for $r \geq 2$. We define the kernel K by $\hat{K}(k) = \chi(|k|) + (1 - \chi(|k|))(-G_h \circ J)^\wedge(k)$. Then $A^{(2)} = -A - A^{(1)}$ has order -2 . We proceed to verify the properties of the symbol a_1 of $A^{(1)}$, which is the sum (4.24). The estimates of Lemma 5.3 show that the sum converges; the sum is positive since the terms are. To show that a_1 is bounded below by $|k|^{-1}$ it is enough to show that $(-G_h \circ J)^\wedge(k) \geq c_1 |k|^{-1}$ for $1 \leq |k| \leq C_0/h$. This can be seen by rewriting (5.11) with $(k, \ell) = |k|(\theta, \xi)$ as

$$(5.23) \quad -(G_h \circ J)^\wedge(|k|\theta) = C|k|^{-1} \int_{-\infty}^{\infty} |M(\theta, \xi)|^{-2} \hat{\psi}(M(\theta, \xi)|k|h) d\xi$$

and recalling that $\hat{\psi}$ is positive and smooth. The estimate for $D_\alpha^s a_1$ follows from the lemma. With regard to the k -difference in (4.10), we note that $i\partial(G_h \circ J)^\wedge/\partial k_\nu$ is the transform of $\alpha_\nu G_h \circ J$. This transform decays like $|k|^{-2}$, according to the lemma. The estimate for $\Delta_{(k)} D_\alpha^s a_1$ follows, bounding k -differences by derivatives for $|k| \geq 2$.

Next we consider the other operators, first ignoring the smooth factor μ and assuming $\hat{x}_j = x_j$. For the operator with kernel $D_x G_h^\pi(x_j - x_\ell)$ the argument above applies for the boundedness, except that the first term in the expansion now has $m = 1, p = 0$, so that the leading operator has order 0. A similar remark applies to $D_x^2 G_h^\pi$. If the factor $\mu(\alpha_j, \alpha_\ell)$ is included, we expand it in the second variable in powers of $\alpha_j - \alpha_\ell$ and incorporate this into the previous expansion, so that there is

no qualitative change. For $\partial G_h^\pi / \partial n(\alpha_\ell) = -n(\alpha_\ell) \cdot \nabla G_h^\pi$, we use a similar expansion for $n(\alpha_\ell)$ in powers of $\alpha_j - \alpha_\ell$. The leading term is $-n(\alpha_j) \cdot \nabla G_h(J(\alpha_j)(\alpha_j - \alpha_\ell))$, and this is zero since G_h is radial and the range of $J(\alpha_j)$ is tangent at α_j ; the remaining operator is of order -1 . In case $\mu = 0$ on the diagonal, the leading term in the expansion of μ is zero. The other terms have at least one factor of $(\alpha_j - \alpha_\ell)$, effectively raising the index p by 1 in each term, and the order of the operator is changed as stated.

Finally we consider the effect of perturbing x_j to \tilde{x}_j . First, using the pointwise estimates (2.4) for derivatives of G_h , we can show that

$$(5.24) \quad \sum_{\ell \in I} |D_x^m G_h^\pi(\tilde{x}_j - \tilde{x}_\ell)| h^2 \leq \begin{cases} C, & |m| = 0, \\ C|\log h|, & |m| = 1, \\ Ch^{-|m|+1}, & |m| = 2, \end{cases}$$

for $|\tilde{x}_j - x_j| \leq c_0 h$, and the same for the sum over j ; see e.g., Lemma 5 of [16] or Lemma 3.2 of [7]. It follows from Young's inequality that the discrete integral operator with kernel $D_x^m G_h^\pi(\tilde{x}_j - \tilde{x}_\ell)$, regarded an operator from L_h^2 to itself, has norm bounded by the right side of (5.24) (e.g., cf. [7], pp. 13-14). The same is true if the kernel is multiplied by a uniformly bounded factor such as μ .

Now suppose the operator with kernel $D_x G_h^\pi(x_j - x_\ell)$ is perturbed by replacing x_j, x_ℓ by $\tilde{x}_j, \tilde{x}_\ell$. The difference of the two kernels can be written as an average of $D_x^2 G_h^\pi$, evaluated along the line from $x_j - x_\ell$ to $\tilde{x}_j - \tilde{x}_\ell$, multiplied by $(\tilde{x}_j - x_j) - (\tilde{x}_\ell - x_\ell)$. If we assume that $\max|\tilde{x}_j - x_j| \leq C_0 h$, then we find, using the above with $|m| = 2$, that the operator on L_h^2 corresponding to this difference is bounded in norm by $Ch^{-1} \cdot h = C$. A similar argument works for the kernel $\mu D_x G_h^\pi(\tilde{x}_j - \tilde{x}_\ell)$, and this verifies the statement in the theorem regarding this operator. It also improves the statement made above for bounds on L_h^2 operators in the case $|m| = 1$, replacing $O(|\log h|)$ by $O(1)$. That is, the norm of the operator on L^2 with kernel $\mu D_x^m G_h^\pi(x_j - x_\ell)$ is $O(1)$ if $|m| = 0, 1$, and $O(h^{-|m|+1})$ if $m \geq 2$. We can now use this improved statement with $|m| = 1$ to verify the assertion that $\mu G_h^\pi(\tilde{x}_j - \tilde{x}_\ell)$ gains one derivative: the error due to the change in the x 's is found to be $O(h)$ as an operator on L^2 , and hE is a bounded operator on L^2 . We can treat the operator $h\mu D_x^2 G_h^\pi$ similarly.

In the special case with $\mu = 0$ on the diagonal, the pointwise estimates for the kernel are better, and we can show that the operator $\mu D_x^2 G_h^\pi(\tilde{x}_j - \tilde{x}_\ell)$ is bounded on L^2 by an argument very similar to that above. We can then use that fact to show that $\mu D_x G_h^\pi(\tilde{x}_j - \tilde{x}_\ell)$ gains one derivative. In turn, this last fact can be used to show that $\mu G_h^\pi(\tilde{x}_j - \tilde{x}_\ell)$ gains two derivatives. \square

Proof of Theorem 5.2. We prove that B_1 is bounded and then remark on B_2 . Let us say that D_h acts in the r -direction, so that e.g., $D_h g$ has transform $h^{-1}\sigma(k_r h)\hat{g}(k)$ for $k \in I$. We will write $\eta(k) = (1 + |k|)^{1/2}$ for the symbol of E . Regarding the sum as an inner product, we can rewrite the operator as

$$(5.25) \quad B_1 f(\alpha_j) = \sum_{\ell \in I} G_h^\pi(x_j - x_\ell) D_{h,r}^* (\mu(\alpha_j, \alpha_\ell) E f(\alpha_\ell)) h^2.$$

We will compare this with

$$(5.26) \quad B_0 f(\alpha_j) = \sum_{\ell \in I} G_h^\pi(x_j - x_\ell) \mu(\alpha_j, \alpha_\ell) D_{h,r}^* E f(\alpha_\ell) h^2.$$

The previous theorem tells us that $G_h^\pi \mu$ gains two derivatives, since $\mu = 0$ on the diagonal, and it follows that B_0 is bounded on L^2 , independent of h . (We think of $D_{h,r}^*$ as E times a bounded operator.) Thus we need only treat the difference of the two operators.

To express $(B_1 - B_0)f$, we write f and μ in Fourier sums:

$$(5.27) \quad f(\alpha_\ell) = \sum_{k \in I} \check{f}(k)e^{ik\ell h}, \quad \mu(\alpha_j, \alpha_\ell) = \sum_{\nu \in I} \check{\mu}(\alpha_j, \nu)e^{i\nu\ell h}.$$

Since μ is assumed smooth, $\check{\mu}(\alpha_j, \nu)$ decays rapidly in ν . Then

$$(5.28) \quad (B_1 - B_0)f(\alpha_j) = \sum_{\nu, \ell} \check{\mu}(\alpha_j, \nu)|\nu|e^{i\nu\ell h} G_h^\pi(x_j - x_\ell) \sum_k b(\nu, k)\eta(k)\check{f}(k)e^{ik\ell h} h^2,$$

where we have set $h^{-1}(\bar{\sigma}((\nu_r + k_r)h) - \bar{\sigma}(k_r h)) = |\nu|b(\nu, k)$. Since we assume σ is continuous with bounded derivative, we have $|\bar{\sigma}((\nu_r + k_r)h) - \bar{\sigma}(k_r h)| \leq Ch|\nu_r|$, so that $b(\nu, k)$ is uniformly bounded. We think of the k -sum as an operator on f and write this as

$$(5.29) \quad (B_1 - B_0)f(\alpha_j) = \sum_{\nu, \ell} \check{\mu}(\alpha_j, \nu)|\nu|e^{i\nu\ell h} G_h^\pi(x_j - x_\ell)(E\Phi_\nu f)(\ell h)h^2,$$

where Φ_ν is defined by $(\Phi_\nu f)^\sim(k) = b(\nu, k)\check{f}(k)$. The operator Φ_ν is bounded on L^2 uniformly in ν as well as h . Finally, we can think of the above as a sum over ν of operators applied to $E\Phi_\nu f$, with kernel $\check{\mu}(\alpha_j, \nu)|\nu|e^{i\nu\ell h} G_h^\pi(x_j - x_\ell)$. Each such operator gains one derivative according to Theorem 5.1, i.e., when composed with E , it gives a bounded operator on L^2 for each ν , with norm depending on the smoothness in (α_j, α_ℓ) of the factor $\check{\mu}(\alpha_j, \nu)|\nu|e^{i\nu\alpha_\ell}$. To sum over ν , we need a bound for some high norm of the factor $e^{i\nu\alpha_\ell}$, and this bound grows with ν . However, assuming μ is smooth enough, $\check{\mu}(\alpha_j, \nu)$ decays so rapidly in ν that the sum is bounded, and we can conclude that $B_1 - B_0$ is bounded on L^2 independent of h .

It suffices to prove the second statement with E^2 replaced by $D_{h,r}$, $r = 1, 2$, since E^2 can be written in terms of these. For this we compare (5.5) with

$$(5.30) \quad \sum_{\ell \in I} D_h G_h^\pi(x_j - x_\ell)\mu(\alpha_j, \alpha_\ell)D_h^* f(\alpha_\ell) h^2.$$

The latter is bounded according to (5.4), and the difference can be treated as in the above argument. □

Finally we need one more fact about sums with $D^m G_h^\pi$:

Lemma 5.4. *Suppose $\mu(\alpha, \alpha')$ is a smooth, periodic function. Let \tilde{x} be a grid function approximating the coordinate mapping x so that $|\tilde{x}(\alpha_j) - x(\alpha_j)| \leq c_0 h$ for each j . Then the sum*

$$(5.31) \quad \sum_{\ell \in I} D^m G_h^\pi(\tilde{x}_j - \tilde{x}_\ell)\mu(\alpha_j, \alpha_\ell)h^2$$

is bounded uniformly in j and h , where m is a multi-index with $|m| = 1$, i.e., D^m denotes any first derivative in x . If $\mu = 0$ when $\alpha = \alpha'$, then the sum is also uniformly bounded for any m with $|m| = 2$.

Proof. The essential point is that, since G_h is radial, DG_h is odd in x and D^2G_h is even. The proofs of the two cases are similar; we prove the second. Only a small neighborhood of the diagonal matters; we assume μ is supported on such a neighborhood and replace G_h^π with G_h . At first we assume \tilde{x} is identical with x . For simplicity we take $j = 0$ and assume $x_0 = x(\alpha_0) = 0$. Since $\mu(0, \alpha) = 0$ at $\alpha = 0$, we can write $\mu(0, \alpha) = \mu_1(\alpha) + \mu_2(\alpha)$, where μ_1 is odd in α and $\mu_2 = O(\alpha^2)$ as $\alpha \rightarrow 0$. Thus, if we replace μ by μ_1 in the sum and average with the sum where ℓ is changed to $-\ell$, we get

$$(5.32) \quad \frac{1}{2} \sum_{\ell \in I} [D^2G_h(x(\alpha_\ell)) - D^2G_h(x(-\alpha_\ell))] \mu_1(\alpha_\ell) h^2 .$$

Since x is smooth, $x(-\alpha) = -x(\alpha) + O(\alpha^2)$, and $D^2G_h(x(-\alpha_\ell)) = D^2G_h(-x(\alpha_\ell)) + R_3$, where the remainder R_3 is $O(\alpha_\ell^2)$ times an average of D^3G_h at points near $x(-\alpha_\ell)$. When we substitute this in the last sum, the D^2G_h terms cancel because of the evenness property. We are left with the sum of $R_3 \mu_1$. This is of order $|\alpha_\ell|^{-1}$ for $\ell \neq 0$, since D^3G_h is of order $|\alpha_\ell|^{-4}$ and μ_1 is of order $|\alpha_\ell|$. This corresponds to an integrable singularity in 2-D, and the sum is bounded independent of h . For the sum with μ_2 , we arrive more directly at a similar estimate, using $\mu_2 = O(|\alpha|^2)$ and $D^2G_h = O(|\alpha|^{-3})$.

To complete the proof, we estimate the change in the sum when x is perturbed to \tilde{x} . Again with $j = 0$, $x(0) = 0$, the change in D^2G_h is $O(h)$ times an average of D^3G_h at points near $x(-\alpha_\ell)$. For some C_1 , $|\tilde{x}(\alpha_\ell)| > h$ and $|x(\alpha_\ell)| > h$ when $|\alpha_\ell| > C_1 h$. Then for such ℓ we again use $D^3G_h = O(|\alpha_\ell|^{-4})$ to bound the resulting sum by

$$(5.33) \quad h \cdot \sum_{\ell \neq 0} |\alpha_\ell|^{-4} |\alpha_\ell| h^2 = h^3 \sum_{\ell \neq 0} |\ell h|^{-3} = C .$$

The remaining ℓ 's are $O(1)$ in number, and it can be checked that their contribution to the sum is $O(1)$. □

6. THE CONVERGENCE PROOF

We now prove that the numerical solution converges to the presumed smooth solution with error $O(h^3)$. As usual we separate consistency and stability, beginning with the former. Assuming an exact solution given, we first compare the velocity v , as computed by the scheme at one time from $x(\alpha_j, t), \phi(\alpha_j, t)$, with the exact velocity. First X_1, X_2 are found at α_j using the discrete operator D_h , and then N, n, X_1^*, X_2^* . The tangential part of v is

$$(6.1) \quad \nabla_h^T \phi = \sum_{k=1,2} (D_{h,k} \phi) X_k^* .$$

The full computed velocity is

$$(6.2) \quad v = \nabla_h^T \phi + wn ,$$

where w is found from the discrete integral equation (1.25), with the operator \mathcal{K}_h defined by (1.26) and f_j by (1.27). The following lemma, proved in §7, concerns the solvability of (1.25).

Lemma 6.1. *Given $x(\alpha, t)$ smooth for $0 \leq t \leq T$, the operator $I + 2\mathcal{K}_h$ is invertible for h sufficiently small, and the norm of $(I + 2\mathcal{K}_h)^{-1}$ as an operator on L_h^2 is bounded uniformly in h and t .*

It is evident that $\nabla_h^T \phi$ and n differ by $O(h^3)$ from the exact values. To compare w with ϕ_n , determined by the harmonic extension of ϕ , we note that ϕ_n satisfies the exact integral equation (1.3). The quadrature results in §3 show that ϕ_n has truncation error $O(h^3)$ in the discrete version (1.25). Then Lemma 6.1 implies that $w - \phi_n = O(h^3)$ at least in L_h^2 . Thus v of (6.2) also differs by $O(h^3)$ from the actual velocity. A similar statement follows for Bernoulli's equation, and in summary the exact solution satisfies the following with $p = 3$:

$$(6.3) \quad x_t = v + O(h^p), \quad \phi_t = \frac{1}{2}|v|^2 - gx_3 + O(h^p) \quad \text{in } L_h^2.$$

It seems that $O(h^3)$ accuracy is not quite enough for simple treatment of the nonlinear terms in the stability estimates. For this reason we use a version of Strang's method (see [26], §5.6). That is, we construct a modification of the exact solution which matches the scheme to higher order, and then compare the computed solution with this modification. The following lemma (proved in §7) asserts that this is possible.

Lemma 6.2. *Suppose $x^{(0)}(\alpha, t), \phi^{(0)}(\alpha, t)$ is a smooth, exact solution of the water wave equations (1.1), (1.2). Then there exist smooth functions $x^{(1)}(\alpha, t), \phi^{(1)}(\alpha, t)$ differing from $x^{(0)}(\alpha, t), \phi^{(0)}(\alpha, t)$ by $O(h^3)$, so that if $v^{(1)}$ is found from $x^{(1)}, \phi^{(1)}$ according to (6.1), (6.2), (1.25)–(1.30), then (6.3) holds for $x^{(1)}, \phi^{(1)}, v^{(1)}$ for any $p < 4$. Also $w^{(1)}$ is within $O(h^3)$ of $\phi_n^{(1)}$ in L_h^2 .*

For the rest of this section we compare quantities such as $v^{(1)}$, found by the scheme from $x^{(1)}, \phi^{(1)}$ at each time, with the corresponding quantities in the computed solution. For simplicity we will drop the superscript (1) for the former. In contrast, we use tildes for the computed solution, determined by

$$(6.4) \quad \tilde{x}_t = \tilde{v}, \quad \tilde{\phi}_t = \frac{1}{2}|\tilde{v}|^2 - g\tilde{x}_3$$

with \tilde{v} found from $\tilde{x}, \tilde{\phi}$ as in (6.1), (6.2), (1.25)–(1.30). We write δx for $\tilde{x} - x$, and similarly for other differences. Thus, e.g., $X_1 = D_{h,1}x, \tilde{X}_1 = D_{h,1}\tilde{x}, \delta X_1 = \tilde{X}_1 - X_1$. Then $\delta v = \tilde{v} - v$ is the error in the computed velocity due to $\delta x, \delta \phi$. Comparing (6.3) and (6.4), we have

$$(6.5) \quad (\delta x)_t = \delta v + O(h^p), \quad (\delta \phi)_t = \frac{1}{2}\delta|v|^2 - g\delta x_3 + O(h^p) \quad \text{in } L_h^2, \quad p < 4.$$

We will show that $\delta x, \delta \phi = O(h^{p-1/2})$ in L_h^2 . With p near 4, it will then follow from the triangle inequality that $\tilde{x}, \tilde{\phi}$ differ from the original exact solution in L_h^2 by $O(h^3)$, thereby completing the proof that the scheme converges.

Our main task now is to express the error δv in computed velocity in terms of $\delta x, \delta \phi$. To do this we need to find the errors in such quantities as $n, \nabla_h^T \phi$, and w . For the latter we vary the integral equation which determines w .

Because we are proving that $\delta x, \delta \phi$ are almost $O(h^{7/2})$ in L_h^2 , we will assume a lower order bound on the errors,

$$(6.6) \quad |\delta x|_{L_h^2} \leq h^3, \quad |\delta \phi|_{L_h^2} \leq h^3, \quad |\delta w|_{L_h^2} \leq h^2, \quad 0 \leq t \leq T.$$

It follows that

$$(6.7) \quad |\delta x|_{L_h^\infty} \leq h^2, \quad |\delta \phi|_{L_h^\infty} \leq h^2, \quad |\delta w|_{L_h^\infty} \leq h, \quad 0 \leq t \leq T.$$

as well as $|\delta D_h x|_{L_h^\infty} \leq C_0 h$, etc. This assumption is helpful in estimating nonlinear terms in the δ 's. It will be removed at the end of the argument.

In order to make use of the gain of derivatives in certain operators related to G_h^π , seen in §5, we will use the discrete Sobolev space H_h^{-1} of grid functions with norm

$$(6.8) \quad |f|_{H_h^{-1}}^2 = \sum_{k \in I} (1 + |k|^2)^{-1} |\check{f}(k)|^2 h^2.$$

We can write $f = E \cdot E^{-1}f$, so that $|E^{-1}f|_{L_h^2} = |f|_{H_h^{-1}}$, with E as in (4.16). Thus if an operator A is of order -1 on L_h^2 , in the language of §5, then A is bounded from H_h^{-1} to L_h^2 , independent of h . In the next lemma we note some facts which will be used.

Lemma 6.3. *We have $|f|_{H_h^{-1}} \leq |f|_{L_h^2}$ and $|f|_{L_h^2} \leq Ch^{-1}|f|_{H_h^{-1}}$ for any f . The operators $D_{h,\ell}$, $D_{h,\ell}^*$ are bounded from L_h^2 to H_h^{-1} , uniformly in h . If ψ is a grid function which either is the restriction of a smooth function or satisfies $|\psi|_{L_h^\infty} \leq Ch$, then $|\psi f|_{H_h^{-1}} \leq C_0|f|_{H_h^{-1}}$, where C_0 depends on ψ but not on h .*

Proof. The first two statements follow from definitions. For the last, we represent elements of H_h^{-1} as differences. Let $D_{h,\ell}^+$ be the first-order forward difference in direction ℓ , $\ell = 1, 2$. Since the Fourier symbol of $D_{h,\ell}^+$ is bounded above and below by $|k_\ell|$ for $k \in I$, we can write any $f \in H_h^{-1}$ as $f = f_0 + D_{h,1}^+ f_1 + D_{h,2}^+ f_2$, where f_0, f_1, f_2 are bounded in L_h^2 by the H_h^{-1} norm of f . Then, e.g., $\psi D_{h,1}^+ f_1 = D_{h,1}^+(\psi f_1) - (D_{h,1}^+ \psi) f_1^\sharp$, where f_1^\sharp is f_1 with a coordinate shift. The factor $D_{h,1}^+ \psi$ is uniformly bounded under either hypothesis on ψ , and it follows that $\psi D_{h,1}^+ f_1$ has the appropriate bound in H_h^{-1} , and in turn the same holds for ψf . \square

Lemma 6.4. *Assume (6.6). Then for the tangent vectors X_ℓ, \tilde{X}_ℓ , $\ell = 1, 2$, we have $|\tilde{X}_\ell - X_\ell|_{H_h^{-1}} \leq C|\tilde{x} - x|_{L_h^2}$. The same is true for the errors in N , $|N|$, n , and X_ℓ^* .*

Proof. The statement for X_ℓ is apparent from the definition of the norm. For the other quantities we use the following general fact: Suppose u is a smooth function of α on the periodic square, possibly vector valued, and suppose \tilde{u}_j is an approximation to $u(\alpha_j)$ such that $|\tilde{u} - u|_{H_h^{-1}} \leq C|\tilde{x} - x|_{L_h^2}$. Assume (6.6), and let F be a smooth function on an open set covering the range of u . Then

$$(6.9) \quad |F(\tilde{u}) - F(u)|_{H_h^{-1}} \leq C' |\tilde{x} - x|_{L_h^2}.$$

The lemma follows from this fact, since the various quantities are functions of X_1, X_2 .

To verify this claim, we first note that, for each α_j ,

$$(6.10) \quad |\tilde{u}_j - u(\alpha_j)| \leq Ch^{-1}|\delta u|_{L_h^2} \leq Ch^{-2}|\delta u|_{H_h^{-1}} \leq Ch^{-2} \cdot h^3 = O(h)$$

by hypothesis, so that \tilde{u} is uniformly close to u . Next, with $u = u(\alpha_j)$, we write $F(\tilde{u}) - F(u) = DF(u)(\delta u) + R(\tilde{u}, u)(\delta u)^2$, where R is an average of the second derivative of F between u and \tilde{u} . The first term is bounded in H_h^{-1} by $C|\delta u|_{H_h^{-1}}$ according to Lemma 6.3, since $DF(u)$ is a smooth factor. For the second term we estimate in L_h^2 . The first factor is uniformly bounded, and for the rest we have

$$(6.11) \quad |(\delta u)^2|_{L_h^2} \leq C|\delta u|_{L_h^\infty} |\delta u|_{L_h^2} \leq Ch|\delta u|_{L_h^2} \leq Ch \cdot h^{-1}|\delta u|_{H_h^{-1}}$$

where we have used (6.10). Thus both terms are bounded by $|\delta u|_{H_h^{-1}} \leq C|\delta x|_{L_h^2}$, and (6.9) is proved. \square

In order to simplify the expressions for errors, we will not be specific about terms contributing to δv which are bounded in L_h^2 by $|\delta x|_{L_h^2}$, $|\delta\phi|_{L_h^2}$, since they do not affect the numerical stability of the scheme. For this reason we use the generic notation $B(f)$ for a grid function which is bounded in L_h^2 , uniformly in h , by $|f|_{L_h^2}$. Thus we write remainders such as $B(\delta x)$, $B(\delta\phi)$.

In the next lemma we find the error in the unit normal, $\delta n = \tilde{n} - n$, due to $\delta x = \tilde{x} - x$, and also the error in the tangential gradient of an arbitrary function μ , defined as in (6.1). Here and below we use the product rule (1.17) for D_h .

Lemma 6.5. *Assuming (6.6), the error in n due to δx is*

$$(6.12) \quad \delta n = -\nabla_h^T(n \cdot \delta x) + B(\delta x).$$

Similarly, if μ is a smooth function of α and $\tilde{\mu}$ is an approximation on the grid, then

$$(6.13) \quad \delta(\nabla_h^T \mu) = \nabla_h^T(\delta\mu) - \nabla_h^T(\delta x \cdot \nabla_h^T \mu) - (\delta n \cdot \nabla_h^T \mu) n + B(\delta x) + B(\delta\mu),$$

$$(6.14) \quad = \nabla_h^T(\delta\mu) - \nabla_h^T(\delta x \cdot \nabla_h^T \mu) + (\nabla_h^T(n \cdot \delta x) \cdot \nabla_h^T \mu) n + B(\delta x) + B(\delta\mu).$$

Proof. Thinking of $n = X_1 \times X_2$ as a pointwise function of $X_k = D_{h,k}x$, $k = 1, 2$, we introduce the infinitesimal change

$$(6.15) \quad \dot{n} = \sum_{k=1,2} (\partial n / \partial X_k) \cdot \delta X_k,$$

where of course $\delta X_k = \tilde{X}_k - X_k$. Then

$$(6.16) \quad \delta n(\alpha_j) = \dot{n}(\alpha_j) + O(|\delta X_k(\alpha_j)|^2).$$

Differentiating $n \cdot n = 1$ shows $\dot{n} \cdot n = 0$, i.e., $\dot{n}(\alpha_j)$ is tangential at $x(\alpha_j)$, and similarly $\dot{n} \cdot X_k = -n \cdot \delta X_k$. Then

$$(6.17) \quad \dot{n} = \sum_{k=1,2} (\dot{n} \cdot X_k) X_k^* = - \sum_{k=1,2} (n \cdot \delta X_k) X_k^*.$$

Now since $\delta X_k = D_{h,k}(\delta x)$, we can write $n \cdot \delta X_k = D_{h,k}(\delta x \cdot n) + B(\delta x)$. Then the above becomes $\dot{n} = -\nabla_h^T(\delta x \cdot n) + B(\delta x)$. We combine this with (6.16) to obtain the result (6.12); the remainder in (6.16) can be estimated in L_h^2 using (6.6) by

$$(6.18) \quad |D_h(\delta x)|_{L_h^\infty} |D_h(\delta x)|_{L_h^2} \leq Ch^{-1} |D_h(\delta x)|_{L_h^2}^2 \leq Ch^{-3} |\delta x|_{L_h^2}^2 \leq C|\delta x|_{L_h^2}.$$

Next we find a similar expression for $\delta X_k^* = \tilde{X}_k^* - X_k^*$. As before, let \dot{X}_k^* be the infinitesimal change in X_k^* due to δx . Again $\delta X_k^* - \dot{X}_k^*$ is quadratic in $D_h(\delta x)$, and it can be estimated as in (6.18). We have $\dot{X}_k^* \cdot X_\ell = -X_k^* \cdot \delta X_\ell$ and $\dot{X}_k^* \cdot n = -X_k^* \cdot \dot{n}$. Then

$$(6.19) \quad \dot{X}_k^* = \sum_{\ell=1,2} (\dot{X}_k^* \cdot X_\ell) X_\ell^* + (\dot{X}_k^* \cdot n) n = - \sum_{\ell=1,2} (X_k^* \cdot \delta X_\ell) X_\ell^* - (X_k^* \cdot \dot{n}) n,$$

and, after moving the ℓ -derivative and replacing \dot{n} ,

$$(6.20) \quad \delta X_k^* = -\nabla_h^T(\delta x \cdot X_k^*) + (\nabla_h^T(n \cdot \delta x) \cdot X_k^*) n + B(\delta x)$$

Finally,

$$(6.21) \quad \delta(\nabla_h^T \mu) = \sum_{k=1,2} D_{h,k}(\delta\mu) X_k^* + (D_{h,k}\mu)\delta X_k^* + D_{h,k}(\delta\mu) \delta X_k^*.$$

The last term can be estimated by $C|\delta\mu|_{L_h^2}$ using (6.6). Combining (6.20), (6.21) we then obtain (6.14), and (6.13) follows. \square

In the next lemma we find an expression for δv in terms of δw .

Lemma 6.6. *With v as in (6.2) and similarly for \tilde{v} , we have, assuming (6.6),*

$$(6.22) \quad \delta v = \nabla_h^T(\delta\phi - v \cdot \delta x) + (\delta w)n - (\delta n \cdot \nabla_h^T\phi)n + B(\delta x) + B(\delta\phi).$$

Proof. Varying (6.2), we have

$$(6.23) \quad \delta v = \delta(\nabla_h^T\phi) + \delta(w n) = \delta(\nabla_h^T\phi) + (\delta w)n + w(\delta n) + (\delta w)(\delta n).$$

From (6.13) we have

$$(6.24) \quad \delta(\nabla_h^T\phi) = \nabla_h^T(\delta\phi) - \nabla_h^T(\nabla_h^T\phi \cdot \delta x) - (\delta n \cdot \nabla_h^T\phi)n + B(\delta x) + B(\delta\phi),$$

and from (6.12)

$$(6.25) \quad w(\delta n) = -w\nabla_h^T(n \cdot \delta x) + B(\delta x) = -\nabla_h^T(w n \cdot \delta x) + B(\delta x).$$

For the last term in (6.23) we can estimate, using (6.6) and Lemma 6.4,

$$(6.26) \quad |(\delta w)(\delta n)|_{L_h^2} \leq C|\delta w|_{L_h^\infty}|\delta n|_{L_h^2} \leq Ch \cdot h^{-1}|\delta n|_{H_h^{-1}} \leq C|\delta x|_{L_h^2}.$$

Now we substitute (6.24)–(6.26) into (6.23). We can combine terms in (6.24), (6.25) using (6.2) to obtain (6.22). \square

The calculation of δv is now reduced to that of δw . To find δw , we subtract the discrete integral equation (1.25) for w from that for \tilde{w} , and obtain an expression with variations in the discrete integrals entering the equation. We state the variations below; they are derived in §7. In the sums, $\nabla G_h^\pi = \nabla G_h^\pi(x_j - x_\ell)$, etc., while in the integrals $\nabla G_h^\pi = \nabla G_h^\pi(x_j - x(\alpha'))$.

$$(6.27) \quad \delta \sum_\ell \nabla G_h^\pi \cdot N_\ell [(n_\ell \cdot n_j)w_\ell - w_j] h^2 = \sum_\ell \nabla G_h^\pi \cdot N_\ell [(n_\ell \cdot n_j)\delta w_\ell - \delta w_j] h^2 + (\delta n_j) \cdot \int (\nabla G_h^\pi \cdot N(x(\alpha'))n(x(\alpha'))\phi_n(\alpha') d\alpha' + hB(\delta w) + B(\delta x),$$

$$(6.28) \quad \delta \sum_\ell \nabla_h^T G_h^\pi \cdot n_j w_\ell |N_\ell| h^2 = \sum_\ell \nabla_h^T G_h^\pi \cdot n_j (\delta w_\ell) |N_\ell| h^2 + \sum_\ell \nabla_h^T G_h^\pi \cdot \nabla_h^T(w_\ell n_\ell \cdot \delta x_\ell) |N_\ell| h^2 + (\delta n_j) \cdot \int \nabla^T G_h^\pi \phi_n(\alpha') |N(\alpha')| d\alpha' + hB(\delta w) + B(\delta x),$$

$$(6.29) \quad \delta \left[n_j \cdot \sum_\ell [D_h G_h^\pi, X]_\ell \times (\nabla_h^T \phi_\ell - \nabla_h^T \phi_j) h^2 - n_j \cdot \sum_\ell \nabla G_h^\pi \cdot N_\ell (\nabla_h^T \phi_\ell - \nabla_h^T \phi_j) h^2 \right] = \sum_\ell \nabla_h^T G_h^\pi \cdot \nabla_h^T (\delta \phi_\ell - \nabla_h^T \phi_\ell \cdot \delta x_\ell) |N_\ell| h^2 + (\delta n_j) \cdot \int \nabla G_h^\pi \times (N(\alpha') \times \nabla^T \phi(\alpha')) d\alpha' + B(\delta x) + B(\delta\phi).$$

When we substitute these into the integral equation for δw , we can collect the terms. The integrals in (6.27) and (6.28) can be combined, and the second sum in (6.28) can be combined with the sum in (6.29) using (6.2). The first terms in (6.27) and (6.28) have the form $\mathcal{K}_h(\delta w)$, with \mathcal{K}_h defined by (1.26), except for

the correction. It can be checked that the error in the correction terms is of type $hB(\delta w) + B(\delta x) + B(\delta\phi)$; the operator $hP_h D_h^*$ is bounded from H_h^{-1} to L_h^2 because of the high k cut-off. Consequently we get

$$(6.30) \quad \left(\frac{1}{2}I + \mathcal{K}_h\right)(\delta w) = \mathcal{L}(\delta\phi - v \cdot \delta x) + (\delta n) \cdot S + hB(\delta w) + B(\delta x) + B(\delta\phi),$$

where the operator \mathcal{L} and the function S are defined by

$$(6.31) \quad (\mathcal{L}f)_j = \sum_{\ell} \nabla_h^T G_h^\pi(x_j - x_\ell) \cdot (\nabla_h^T f)_\ell |N_\ell| h^2,$$

$$(6.32) \quad S_j = \int \nabla G_h^\pi \times (N(\alpha') \times \nabla^T \phi(\alpha')) d\alpha' - \int \nabla G_h^\pi \phi_n(\alpha') |N(\alpha')| d\alpha'.$$

Lemma 6.1 assures us that (6.30) can be solved for δw ; the solvability is not affected by the small term $hB(\delta w)$. The following related lemma guarantees that \tilde{w} can be found from its discrete integral equation.

Lemma 6.7. *Under assumption (6.6) the operator $I + 2\tilde{\mathcal{K}}_h$, obtained by replacing x with \tilde{x} in (1.26), is invertible for h sufficiently small, and the operator norm of the inverse is uniformly bounded. The discrete integral equation can be solved by the simple iteration (1.34).*

The principal part of the operator \mathcal{L} is of central importance in estimating the growth of numerical error. The following lemma identifies this principal part and its properties.

Lemma 6.8. *The operator \mathcal{L} on L_h^2 defined by (6.31) has the form $\mathcal{L} = \frac{1}{2}\Lambda + B_0$, where B_0 is bounded on L_h^2 , uniformly in h , and Λ is an operator with the following properties:*

(i) Λ is self-adjoint as an operator on L_h^2 , Λf is real-valued for real f , and

$$(6.33) \quad (\Lambda f, f)_{L_h^2} \geq c_0 |E^{1/2} f|_{L_h^2}^2 = c_0 \sum_{k \in I} (1 + |k|^2)^{1/2} |\check{f}(k)|^2.$$

(ii) There are operators B_1, \dots, B_5 , bounded on L_h^2 , uniformly in h , so that

$$(6.34) \quad \Lambda = B_1 E, \quad \Lambda = E B_2,$$

$$(6.35) \quad \Lambda = E^{1/2} B_3 E^{1/2}, \quad E = B_4 \Lambda + B_5.$$

Here E is the absolute derivative defined in (4.16).

Proof. The result depends on the assumptions (1.14)–(1.16) for D_h , as well as the positivity of $-\tilde{G}_h$. If we write out ∇_h^T , we have

$$(6.36) \quad \mathcal{L}f(\alpha_j) = - \sum_{\ell, \mu, \nu} D_{h, \mu} G_h^\pi(x_j - x_\ell) (D_{h, \nu} f)_\ell (X_{\mu\ell}^* \cdot X_{\nu\ell}^*) |N_\ell| h^2$$

with $\mu, \nu = 1, 2$, or, after summing by parts and setting $b_\ell^{\mu\nu} = (X_{\mu\ell}^* \cdot X_{\nu\ell}^*) |N_\ell| = (g^{\mu\nu})_\ell |N_\ell|$,

$$(6.37) \quad \mathcal{L}f(\alpha_j) = - \sum_{\ell, \mu, \nu} G_h^\pi D_{h, \mu}^* [b_\ell^{\mu\nu} D_{h, \nu} f] h^2 = - \sum_{\ell, \mu, \nu} G_h^\pi b_\ell^{\mu\nu} D_{h, \mu}^* D_{h, \nu} f h^2 + (Bf)(\alpha_j).$$

To see that the remainder is bounded, we use (1.17) for $D_{h, \mu}^*$ and note that the operator with kernel G_h^π , times a smooth factor, is of order -1 , according to Theorem 5.1. Next we replace $b_\ell^{\mu\nu}$ with $b_j^{\mu\nu}$; the difference is an operator applied to

$D_{h,r}^* D_{h,\nu} f$ with the kernel G_h^π times a function which vanishes at $\ell = j$. This operator has order -2 , by Theorem 5.1, and so the error is again bounded in f . We now have

$$(6.38) \quad \mathcal{L}f(\alpha_j) = - \sum_{\mu,\nu} b_j^{\mu\nu} (AD_{h,\mu}^* D_{h,\nu} f)(\alpha_j) + (Bf)(\alpha_j),$$

where A is the operator of Theorem 5.1, with kernel G_h^π . There we wrote A as $A = -A^{(1)} - A^{(2)}$, where $A^{(2)}$ is of order -2 , and thus contributes a bounded term to \mathcal{L} , while $A^{(1)}$ is an operator of type (4.2) whose symbol $a_1(\alpha, k)$ is of class S^{-1} with $a_1(\alpha, k) \geq c_1(1 + |k|^2)^{-1/2}$ for $k \in I$. Thus $\mathcal{L} = \Lambda_0 + B$, where Λ_0 is the operator of type (4.2) with symbol λ_0 of class S^1 ,

$$(6.39) \quad \lambda_0(\alpha, k) = h^{-2} a_1(\alpha, k) \sum_{\mu,\nu} b^{\mu\nu}(\alpha) \bar{\sigma}(k_\mu h) \sigma(k_\nu h).$$

We have $\lambda_0(-k) = \bar{\lambda}_0(k)$, which implies that Λ_0 preserves real functions. Since the matrix $b^{\mu\nu}$ is positive definite and symmetric, and $h^{-1} |\sigma(k_\mu h)| \geq C|k_\mu|$ for $k \in I$, we have $\lambda_0(\alpha, k) \geq c_2|k|$ for $k \in I$. Thus Lemma 4.5 applies to Λ_0 ; the estimate (4.18) holds for Λ_0 , and $\Lambda_0^* - \Lambda_0$ is bounded. Now we set $\Lambda = \Lambda_0^* + \Lambda_0 + C_0$, where C_0 is a large enough constant. Then $\Lambda - 2\Lambda_0$ is bounded, and the properties of Λ follow from Lemmas 4.4–4.6. □

In view of this lemma, equation (6.30) reduces to

$$(6.40) \quad (I + 2\mathcal{K}_h)(\delta w) = \Lambda(\delta\phi - v \cdot \delta x) + 2(\delta n) \cdot S + hB(\delta w) + B(\delta x) + B(\delta\phi).$$

We now show that the term $\mathcal{K}_h(\delta w)$ is negligible. The two main terms on the right above can be written as $Ef + B(\delta x) + B(\delta\phi)$ for some f with $|f|_{L_h^2} \leq C(|\delta x|_{L_h^2} + |\delta\phi|_{L_h^2})$; this follows from (6.12) and (6.34). Then δw is $(I + 2\mathcal{K}_h)^{-1}Ef$ plus a remainder, and the main term in $\mathcal{K}_h(\delta w)$ is $(I + 2\mathcal{K}_h)^{-1}\mathcal{K}_hEf$. By Lemma 6.1, the last is bounded in L_h^2 norm by $|\mathcal{K}_hEf|_{L_h^2}$. Theorems 5.1 and 5.2 imply that the operator \mathcal{K}_h is of order -1 ; for the second term in \mathcal{K}_h we use the fact that $X_{k\ell}^* \cdot n_j = 0$ when $\ell = j$. Thus $|\mathcal{K}_hEf|_{L_h^2} \leq C|f|_{L_h^2}$, and it follows that $\mathcal{K}_h(\delta w) = hB(\delta w) + B(\delta x) + B(\delta\phi)$. We can now absorb $\mathcal{K}_h(\delta w)$ into the remainder in (6.40), and then invert $(I + hB)$ acting on δw , simplifying (6.40) to

$$(6.41) \quad (\delta w) = \Lambda(\delta\phi - v \cdot \delta x) + 2(\delta n) \cdot S + B(\delta x) + B(\delta\phi).$$

Next we substitute (6.41) into (6.22) to find a definitive expression for δv . After combining we have

$$(6.42) \quad \delta v = \nabla_h^T(\delta\phi - v \cdot \delta x) + \Lambda(\phi - v \cdot \delta x)n + \delta n \cdot (2S - \nabla^T\phi)n + B(\delta x) + B(\delta\phi).$$

(We have replaced $\nabla_h^T\phi$ with the exact $\nabla^T\phi$, at a cost of $hB(\delta n) = B(\delta x)$.) However, the third term above is negligible, as a consequence of potential theory: If Φ is a periodic harmonic function below the surface $x(\alpha)$, then

$$(6.43) \quad 2 \int \nabla^{T(x)} G^\pi \times (n(y) \times \nabla^T \Phi(y)) dS(y) - 2 \int \nabla^{T(x)} G^\pi \frac{\partial \Phi}{\partial n(y)} dS(y) - \nabla^T \Phi(x) = 0,$$

where $G^\pi = G^\pi(x - y)$ and $\nabla^{T(x)}$ means the part of the gradient which is tangential at x . This follows from the same argument as for the integral equation (1.3), except that we take the limiting tangential derivative at the surface. If we replace G^π by

G_h^π , Φ by ϕ , and $\partial\Phi/\partial n$ by w , the above holds with error $O(h)$, because of the regularization of G and the modification in Lemma 6.2. The resulting expression almost matches $2S - \nabla^T \phi$, except that the latter has ∇G^π rather than $\nabla^{T(x)} G^\pi$. But δn is tangential except for a $B(\delta x)$ term; see (6.12). Therefore $\delta n \cdot (2S - \nabla^T \phi)$ has the form $hB(\delta n) + B(\delta x)$ and thus $B(\delta x)$. In summary, we have

$$(6.44) \quad \delta v = \nabla_h^T (\delta\phi - v \cdot \delta x) + \Lambda(\delta\phi - v \cdot \delta x)n + B(\delta x) + B(\delta\phi).$$

We want to replace the discrete approximation v in (6.44) with x_t , the actual velocity of the modified exact solution. From (6.3) we see that $x_t - v$ is $O(h^p)$ in L_h^2 and thus $O(h^{p-1})$ in L_h^∞ . The change in δv is then $h^{p-2}(B(\delta x) + B(\delta\phi))$. Since $p > 2$, this can be absorbed into the remainder. Thus we introduce

$$(6.45) \quad u_1 = \delta\phi - x_t \cdot \delta x$$

and rewrite (6.44) as

$$(6.46) \quad \delta v = \nabla_h^T u_1 + (\Lambda u_1)n + B(\delta x) + B(\delta\phi).$$

We are now ready to estimate the growth in time of the errors in $\delta x, \delta\phi$. Because of the special structure of δv in (6.46), we can use an argument similar to that in [5], [6]. We will replace $\delta x, \delta\phi$ by new state variables u_1, u_2, u_3 , where u_1 is defined by (6.45) and

$$(6.47) \quad u_2 = \delta x \cdot n,$$

so that, recalling (6.5), we have in L_h^2

$$(6.48) \quad \begin{aligned} u_{2,t} &= (\delta x)_t \cdot n + B(\delta x) = \delta v \cdot n + B(\delta x) + O(h^p) \\ &= \Lambda u_1 + B(\delta x) + B(\delta\phi) + O(h^p). \end{aligned}$$

We will choose u_3 to account for $(\delta x)^T$ while taking advantage of the similarity of the two main terms in (6.46). We will need to know that B_4 of Lemma 6.8, and later also B_3 , have bounded time derivatives. This follows from their construction in §4 once we know that the t -derivative of the symbol $a_1(\alpha, k; h)$ in Theorem 5.1 has bounds similar to those for a_1 itself, i.e., as a symbol of class S^{-1} . The essential point is that $G_h(J\alpha)$ depends on t only through the Jacobian J , and its transform through the related matrix M (see (5.11)); differentiation in t does not change the degree of homogeneity in α or k , and the estimates for G_h^π apply to $\partial G_h^\pi/\partial t$ as well.

To define u_3 , we first write $\nabla_h^T = B_6\Lambda + B_7$, using (6.35), with B_6, B_7 bounded uniformly in h, t , determined by B_4, B_5 . We now define

$$(6.49) \quad u_3 = (\delta x)^T - B_6(\delta x \cdot n).$$

Applying $\partial/\partial t$, using the boundedness of $B_{6,t}$, and dropping less important terms, we find that

$$(6.50) \quad \begin{aligned} u_{3,t} &= (\delta v)^T - B_6(\delta v \cdot n) + B(\delta x) + O(h^p) \\ &= \nabla_h^T u_1 - B_6(\Lambda u_1) + B(\delta x) + O(h^p) = B(\delta x) + B(\delta\phi) + O(h^p), \end{aligned}$$

with no important terms remaining.

Next we derive the equation for $u_{1,t}$. From (6.5) we obtain

$$(6.51) \quad \delta\phi_t = \frac{1}{2}\delta(v \cdot v) - g\delta x_3 + O(h^p) = v \cdot \delta v + \frac{1}{2}|\delta v|^2 - g\delta x_3 + O(h^p).$$

For the other term in u_1 we have

$$(6.52) \quad (x_t \cdot \delta x)_t = x_t \cdot \delta v + x_{tt} \cdot \delta x + O(h^p).$$

When we subtract, we have a term $(v - x_t)\delta v$. From (6.5), $v - x_t = O(h^{p-1})$ in L_h^∞ , and from (6.46) δv has the form $h^{-1}(B(\delta x) + B(\delta\phi))$. Then this term is $h(B(\delta x) + B(\delta\phi))$, since $p > 3$. Combining terms, we have

$$(6.53) \quad u_{1,t} = -(x_{tt} + ge_3) \cdot \delta x + \frac{1}{2}|\delta v|^2 + hB(\delta x) + hB(\delta\phi) + O(h^p).$$

For an exact solution of the Euler equations, $-(x_{tt} + ge_3) = \nabla p$, the pressure gradient. At the water surface, this is a normal vector, since $p = 0$ there. Moreover, we saw in (1.35) that $-\nabla p \cdot n \geq c_0 > 0$ at the surface. We have modified the exact solution by $O(h^3)$, and thus in our case we have

$$(6.54) \quad x_{tt} + ge_3 = -cn + O(h^3), \quad c = c(\alpha, t) \geq c_0 > 0.$$

The first term in (6.53) is thus $-c\delta x \cdot n + h^3B(\delta x) = -cu_2 + h^3B(\delta x)$. We need an estimate for the $(\delta v)^2$ term in (6.53). From (6.46) and (6.6) we have $|\delta v|_{L_h^\infty} = O(h)$, and also $|\delta v|_{L_h^2} \leq C|Eu_1|_{L_h^2} \leq h^{-1/2}|E^{1/2}u_1|_{L_h^2}$, and combining these two facts, $|(\delta v)^2|_{L_h^2} \leq h^{1/2}|E^{1/2}u_1|_{L_h^2}$.

We can now estimate the growth of a norm of (u_1, u_2, u_3) . We define a norm so that the two principal terms will cancel in the growth estimates,

$$(6.55) \quad U = \frac{1}{2}\{(\Lambda u_1, u_1)_{L_h^2} + |c^{1/2}u_2|_{L_h^2}^2 + |c^{1/2}u_3|_{L_h^2}^2\} \equiv U_1 + U_2 + U_3.$$

We have

$$(6.56) \quad |\delta x|_{L_h^2}^2 + |\delta\phi|_{L_h^2}^2 \leq CU, \quad |E^{1/2}u_1|_{L_h^2}^2 \leq CU,$$

and we can rewrite our equations as

$$(6.57) \quad u_{1,t} = -cu_2 + h^{1/2}r_1 + h^p\tau_1, \quad u_{2,t} = \Lambda u_1 + r_2 + h^p\tau_2, \quad u_{3,t} = r_3 + h^p\tau_3,$$

where the r 's are bounded in L_h^2 by $U^{1/2}$, and the τ 's by a constant. Then

$$(6.58) \quad U_{1,t} = (u_{1,t}, \Lambda u_1) + \frac{1}{2}(\Lambda_t u_1, u_1) \\ = -(cu_2, \Lambda u_1) + h^{1/2}(r_1, \Lambda u_1) + \frac{1}{2}(B_{3,t}E^{1/2}u_1, E^{1/2}u_1) + h^p(\tau_1, \Lambda u_1).$$

The second term can be estimated by

$$(6.59) \quad Ch^{1/2}|r_1|_{L_h^2}|Eu_1|_{L_h^2} \leq Ch^{1/2}|r_1|_{L_h^2} h^{-1/2}|E^{1/2}u_1|_{L_h^2} \leq CU$$

and the third term by $C|E^{1/2}u_1|_{L_h^2}^2 \leq CU$. Recalling that $\Lambda = B_1E$, we estimate the last term by

$$(6.60) \quad Ch^p|\Lambda u_1|_{L_h^2} \leq Ch^p|Eu_1|_{L_h^2} \leq Ch^{p-1/2}|E^{1/2}u_1|_{L_h^2} \leq Ch^{p-1/2}U^{1/2},$$

and in summary

$$(6.61) \quad U_{1,t} = (u_{1,t}, \Lambda u_1) + R_1, \quad |R_1| \leq C(U + h^{p-1/2}U^{1/2}).$$

For U_2 we have

$$(6.62) \quad U_{2,t} = (cu_{2,t}, u_2) + \frac{1}{2}(c_t u_2, u_2) = (c\Lambda u_1, u_2) + R_2$$

with $|R_2|$ bounded by $C(U + h^pU^{1/2})$, and similarly $U_{3,t} = R_3$. When we add, the two main terms in (6.61), (6.62) cancel, and we have $U_t \leq C_1(U + h^{2p-1})$. Then $U(t) \leq C_2h^{2p-1}$ for $0 \leq t \leq T$, and from (6.56)

$$(6.63) \quad |\delta x|_{L_h^2} + |\delta\phi|_{L_h^2} \leq C_3h^{p-1/2}, \quad 0 \leq t \leq T.$$

It follows from (6.46) and Lemma 6.6 that

$$(6.64) \quad |\delta v|_{L_h^2}, |\delta w|_{L_h^2} \leq C_4 h^{p-3/2}, \quad 0 \leq t \leq T.$$

We can now remove the assumption (6.6) used to derive (6.63), (6.64). We can take p near 4, so that $p - 1/2$ is almost $7/2$. For h small enough, (6.63), (6.64) imply that the L_h^2 norms of $\delta x, \delta \phi, h\delta w$ remain below $h^3/2$ as long as they are less than h^3 , and therefore they never reach h^3 . Thus for small h (6.63), (6.64) hold without qualification, and in view of Lemma 6.2 the computed solution stays within $O(h^3)$ of the actual solution in L_h^2 .

7. PROOFS OF LEMMAS

Here we present the proofs of Lemma 6.1, Lemma 6.2, estimates (6.27)–(6.29), and Lemma 6.7.

Proof of Lemma 6.1. The invertibility of $I + 2\mathcal{K}_h$ will follow from that of the operator $I + 2\mathcal{K}$ of which it is an approximation, where \mathcal{K} is the operator acting on periodic functions of α ,

$$(7.1) \quad \mathcal{K}f(\alpha) = \int \nabla G^\pi(x(\alpha) - x(\alpha')) \cdot n(x(\alpha)) f(\alpha') |N(\alpha')| d\alpha'.$$

Thus $\mathcal{K}f$ is the adjoint double layer potential due to f . With time t fixed for the moment, the operator \mathcal{K} is compact, as an operator on L^2 of the periodic square, so that its nonzero spectrum consists only of eigenvalues. Classical arguments show that the operator $2\mathcal{K}$ and its adjoint $2\mathcal{K}^*$ have spectral radius strictly less than 1; that is, if λ is an eigenvalue of $2\mathcal{K}$, then $|\lambda| \leq \rho(2\mathcal{K}) < 1$. This fact depends on the periodic geometry; for bounded domains there is an eigenvalue with $|\lambda| = 1$. A proof that $\rho(2\mathcal{K}) = \rho(2\mathcal{K}^*) < 1$ was given in [3] for double layer potentials in periodic regions in two dimensions; essentially the same proof applies to the present case of 3-D regions with doubly periodic boundaries.

Now let $\mathcal{K}(t)$ be the operator at time t for $0 \leq t \leq T$. We argue that for some constants $\varepsilon > 0$ and $C_0 > 0$, and for all complex λ with $|\lambda| \geq 1 - \varepsilon$, and all t with $0 \leq t \leq T$, the operator $\lambda I - 2\mathcal{K}(t)$ is invertible, and $\|(\lambda I - 2\mathcal{K}(t))^{-1}\| \leq C_0$. First, since $\rho(2\mathcal{K}(t)) < 1$, then also $\rho(2\mathcal{K}(t) + A) < 1$ if A is small enough in norm as an operator on L^2 ; this is shown in [10], Theorem 1.37. It can be checked that $\mathcal{K}(t)$ depends continuously on t , as an operator on L^2 , using the smoothness assumptions. Thus the above statement tells us that for each t_0 there is a t -interval near t_0 such that $\rho(2\mathcal{K}(t))$ is bounded away from 1 on the interval. Since $[0, T]$ is a compact set, the same is true for this entire interval, i.e., there is some $\varepsilon > 0$ so that $\rho(2\mathcal{K}(t)) < 1 - \varepsilon$ for each $t \in [0, T]$. This shows that $\lambda I - 2\mathcal{K}(t)$ is invertible for each t and λ with $|\lambda| \geq 1 - \varepsilon$. The inverse depends continuously on t, λ , and so a uniform bound for the norm follows for λ in a bounded set by compactness. Finally, we have a uniform bound for the norm of $\mathcal{K}(t)$, and from this we can easily obtain a bound for the inverse for large λ . This verifies the assertion.

The above fact allows us to show that operators close to $\mathcal{K}(t)$ have similar properties. Suppose A is any operator on L^2 with $\|A\| < (2C_0)^{-1}$, where C_0 is as above. Then for any t and any λ with $|\lambda| \geq 1 - \varepsilon$, we have $\lambda I - (2\mathcal{K} - A) = (\lambda I - 2\mathcal{K})[I + (\lambda I - 2\mathcal{K})^{-1}A]$. By the statement above, each of the last two factors is invertible, and the inverse has norm bounded by $2C_0$. Thus we have shown that $\rho(2\mathcal{K}(t) - A) < 1 - \varepsilon$, and in particular $\|(I + 2\mathcal{K}(t) - A)^{-1}\| \leq 2C_0$. To complete

the proof of the lemma, it will be sufficient to show that \mathcal{K}_h can be regarded as a small perturbation of \mathcal{K} when h is small.

We first treat the operator \mathcal{K}_h^0 , which is \mathcal{K}_h with the two terms with w_j omitted. To show that $I + 2\mathcal{K}_h^0$ is invertible on L_h^2 , we identify it with an operator on $L^2([-\pi, \pi]^2)$; i.e., we extend from the discrete variable $\alpha_j \in Ih$ to $\alpha \in [-\pi, \pi]^2$. We partition the square by defining $B_j = \{\alpha \in [-\pi, \pi]^2 : 0 \leq \alpha_\nu - (\alpha_j)_\nu < h, \nu = 1, 2\}$ for $j \in I$. If we write \mathcal{K}_h^0 in the form

$$(7.2) \quad \mathcal{K}_h^0 f(\alpha_j) = \sum_{\ell \in I} K_h(\alpha_j, \alpha_\ell) f(\alpha_\ell) h^2,$$

we can extend the kernel by defining $K_h(\alpha, \alpha') = K_h(\alpha_j, \alpha_\ell)$ for $\alpha \in B_j, \alpha' \in B_\ell$. This kernel then gives an integral operator on $L^2([-\pi, \pi]^2)$. Now if f is a function on Ih , we can extend it to a piecewise constant function on $[-\pi, \pi]^2$ by defining $f(\alpha) = f(\alpha_\ell)$ for $\alpha \in B_\ell$. The integral operator applied to this extended f produces a piecewise constant function with values given by (7.2). The L^2 norms of the extended f and its image match the L_h^2 norms of the discrete functions. (Cf. [6], Lemma 5; [7], p. 16.) Thus if we show that the extended operator $I + 2\mathcal{K}_h^0$ has an inverse, bounded independent of h , then the same will be true for the discrete operator.

In view of the above remarks, it will be sufficient to show that the discrete operator \mathcal{K}_h^0 , when extended, is close to the corresponding continuous version. The two terms of \mathcal{K}_h^0 have the form

$$(7.3) \quad J_1 f(\alpha_j) = \sum_{\ell \in I} N_\ell \cdot \nabla G_h^\pi(x_j - x_\ell) \mu_1(\alpha_j, \alpha_\ell) f(\alpha_\ell) h^2,$$

$$(7.4) \quad J_2 f(\alpha_j) = \sum_{\ell \in I} D_h G_h^\pi(x_j - x_\ell) \mu_2(\alpha_j, \alpha_\ell) f(\alpha_\ell) h^2,$$

where μ_1, μ_2 are smooth, μ_2 is zero on the diagonal, D_h is the discrete derivative with respect to α_ℓ , and N_ℓ is computed from $x(\alpha)$ using D_h . Thus, in the first case, we compare J_1 extended to L^2 with

$$(7.5) \quad \int N(\alpha') \cdot \nabla G_h^\pi(x(\alpha) - x(\alpha')) \mu_1(\alpha, \alpha') f(\alpha') d\alpha'.$$

(We have already seen in Theorem 2.3 that the change in the integral due to regularizing G to G_h is $O(h^3)$.) The error to be accounted for is that from replacing $x(\alpha)$ by $x_j, x(\alpha')$ by x_ℓ , and $N(\alpha')$ by N_ℓ in the kernel when $\alpha \in B_j, \alpha' \in B_\ell$. We use an estimate for the first derivative of the kernel. We consider G_h instead of G_h^π , since the remainder is smooth. Since G_h is radial, we have

$$(7.6) \quad N(\alpha') \cdot \nabla G_h(x(\alpha) - x(\alpha')) = |x(\alpha) - x(\alpha')|^{-1} \frac{\partial G_h}{\partial r} [N(\alpha') \cdot (x(\alpha) - x(\alpha'))].$$

The last factor is $O(|\alpha - \alpha'|^2)$ for α near α' , since $x(\alpha) - x(\alpha')$ is almost tangent. From the estimates (2.4) for G_h , we have $|(\partial/\partial r)^m G_h| \leq C|\alpha - \alpha'|^{-m-1}$ for $|\alpha - \alpha'| \geq h$ and $O(h^{-m-1})$ otherwise, where $m = 1$ or 2 . Combining these facts, we find for the kernel $K(\alpha, \alpha')$ of (7.5) that $|DK(\alpha, \alpha')| \leq C|\alpha - \alpha'|^{-2}$ for $|\alpha - \alpha'| \geq h$ and $O(h^{-2})$ otherwise; here D denotes a first derivative in α or α' . Thus the error in discretizing the kernel is of order $h \cdot h^{-2}$ for α, α' close, and order $h \cdot |\alpha - \alpha'|^{-2}$ when they are at least $O(h)$ apart. We can estimate the norm of the operator resulting from this error just as in the last part of the proof of Theorem 5.1; the

norm is bounded by $Ch|\log h|$. Replacing $N(\alpha_\ell)$ with N_ℓ leads to a smaller error, since they differ by $O(h^3)$.

We argue similarly for the second operator J_2 . We need to compare the kernel $\mu_2 DG_h^\pi(x(\alpha) - x(\alpha'))$ with discrete values of $\mu_2 D_h G_h^\pi$. (Again the change in the integral from regularizing G to G_h is $O(h^3)$.) Assuming first that D_h is a difference operator, the error in replacing $DG_h^\pi(x_j - x_\ell)$ with $D_h G_h^\pi(x_j - x_\ell)$ can be estimated by writing $(D_h - D)G_h^\pi$ as an integral of $D^2 G_h^\pi$. This is controlled by a bound for $h \cdot D^2 G_h^\pi$ on an $O(h)$ neighborhood of $x_j - x_\ell$. Since $\mu_2(\alpha_j, \alpha_\ell) = 0$, we find that the contribution to the error in the kernel is then of order $h \cdot |\alpha_j - \alpha_\ell|^{-2}$ when α_j, α_ℓ are apart, and of order h^{-1} when they are close. Just as before, this estimate leads to an error in the operator with norm of order $h|\log h|$. Next we assess the error in discretizing $\mu_2 DG_h^\pi$. The error in the kernel has terms of the form $h \cdot \mu_2 D^2 G_h^\pi$ and $h \cdot DG_h^\pi$. For either of these we obtain the same estimates as before, using again the fact that $\mu_2 = 0$ on the diagonal. This completes the treatment of J_2 if D_h is a difference operator. If not, we can reduce to the special case by comparing the discrete $\mu_2 D_h G_h^\pi$ with one where D_h is replaced by a difference operator. For this we note that $D_h^{(1)} - D_h^{(2)}$ has the form hBE^2 for some bounded B , and by Theorem 5.2 and (5.5), the two operators differ by $O(h)$.

In summary, we have shown that the error in discretizing each operator J_1, J_2 is $O(h|\log h|)$, and thus $\mathcal{K}_h^0 - \mathcal{K}$ is of the same order. Finally we consider $\mathcal{K}_h - \mathcal{K}_h^0$. Each of the two terms multiplies w_j by a factor. For the correction term this factor is $O(h)$; for the other term it is a sum which is within $O(h)$ of the first integral in (1.5), which is zero. Thus $\mathcal{K}_h - \mathcal{K}_h^0$ is $O(h)$, and therefore $\mathcal{K}_h - \mathcal{K}$ is $O(h|\log h|)$, as operators on L_h^2 . □

Proof of Lemma 6.2. The exact equations for x, ϕ , as functions of α, t , have the form $x_t = v, \phi_t = |v|^2/2 - gx_3$, with v determined by $v = \nabla^T \phi + wn$, and with $(\frac{1}{2}I + \mathcal{K}(x))w = f(x, \phi)$. We think of this system in the form $z_t = F(z)$, where $z = (x, \phi)$ and F is a nonlocal mapping. Let H^s be the Sobolev space of scalar-valued periodic functions of α with s derivatives in L^2 , X^s the space of such vector-valued functions, and Z^s the space of pairs $x \in X^s, \phi \in Y^s$. We choose $s_0 > 1$ and check that F is C^2 from Z^{s_1} to Z^{s_0} when s_1 is large enough relative to s_0 . First, the single and double layer potentials define bounded operators from H^{s_0} to H^{s_0+1} , and they are at least C^2 as functions of $x \in X^{s_1}$; the x -derivatives do not change the order of the singularity. Then $f : Z^{s_1} \rightarrow H^{s_0}$ is C^2 . Since $I + 2\mathcal{K}$ is a Fredholm operator on H^{s_0} and is 1-1, it is invertible, and the inverse is a C^2 function of $x \in X^{s_1}$. It now follows easily that $F : Z^{s_1} \rightarrow Z^{s_0}$ is C^2 .

We need to use $DF(z^0)$, the derivative of F at the exact, smooth solution z^0 . We presume that z^0 exists in Z^{s_2} for some s_2 larger than s_1 . Finding $DF(z^0)$ amounts to linearizing the equations about z^0 , and this can be done as for the discrete equations in §6 but more easily. Writing the infinitesimal variation in z in the u variables of (6.45), we have $DF(z^0)u = (-cu_2, \Lambda u_1, 0) + (0, B_2 u, B_3 u)$, where Λ is a positive pseudodifferential operator of order 1 and B_2, B_3 are bounded in H^{s_1} by $u_2, u_3 \in H^{s_1}$. For solutions of $u_t = DF(z^0)u$, we can estimate as in §6 but in high norms. Let $U_m = (\Lambda D^m u_1, D^m u_1)_{L^2} + |D^m(c^{1/2}u_2)|_{L^2}^2 + |D^m(c^{1/2}u_3)|_{L^2}^2$ where m is a multi-index for the α -derivative D , and let $U = \Sigma U_m, |m| \leq s_1$. Then $U_t \leq C_1 U$, and thus $U(t) \leq C_2 U(0)$ for $0 \leq t \leq T$. (Cf. [5], p. 1282.)

The discrete equations have a similar structure $z_{h,t} = F_h(z_h)$, with v_h determined by w_h satisfying $(\frac{1}{2}I + \mathcal{K}_h(x_h))w_h = f_h(z_h)$. The consistency argument shows

that for any $z = (x, \phi) \in Z^{s_1}$ we have $(\frac{1}{2}I + \mathcal{K}_h(x))\phi_n = f_h(z) + h^3 r_{31}(z) + r_{41}(z, h)$, where $r_{31}(z) \in H^{s_0}$, depending smoothly on $z \in Z^{s_1}$, and r_{41} is uniformly $O(h^4)$. To invert, we use the fact that $(\frac{1}{2}I + \mathcal{K}_h(x))^{-1}$ differs as an operator on L^2 from $(\frac{1}{2}I + \mathcal{K}(x))^{-1}$ by $O(h|\log h|)$, as shown in the proof of Lemma 6.1. Thus we can write $\phi_n = (\frac{1}{2}I + \mathcal{K}_h(x))^{-1}f_h(z) + h^3 r_{32}(z) + r_{42}(z, h)$, where $r_{32}(z) = (\frac{1}{2}I + \mathcal{K}(x))^{-1}r_{31}(z)$ depends smoothly in H^{s_0} on z as above, and r_{42} is bounded in L_h^2 by $Ch^4|\log h|$. (The $\log h$ can be removed by a more careful argument.) Similarly, for any $z \in Z^{s_1}$, we get $F(z) - F_h(z) = h^3 r_3(z) + r_4(z, h)$, where $r_3 : Z^{s_1} \rightarrow Z^{s_0}$ is smooth and $r_4(z, h)$ is $O(h^4|\log h|)$ in L_h^2 . We can also assume that $r_3(z^0) \in Z^{s_1}$, since $z^0 \in Z^{s_2}$.

Now we can combine the above to modify z^0 . First, we can solve the linear equation $\eta_t = DF(z^0)\eta - r_3(z^0)$, $\eta = 0$ at $t = 0$, with $\eta \in Z^{s_1}$; this can be done in a standard way from the linear estimate above. Now set $z^1 = z^0 + h^3\eta$ in Z^{s_1} . Then $F(z^1) = F(z^0) + h^3 DF(z^0)\eta + O(h^6)$ in Z^{s_0} , since F is C^2 . We check that z^1 has the desired property. We have $z_t^1 = F(z^0) + h^3 DF(z^0)\eta - h^3 r_3(z^0) = F(z^1) - h^3 r_3(z^0) + O(h^6) = F_h(z^1) - h^3 r_3(z^0) + O(h^6) + h^3 r_3(z^1) + r_4(z^1, h)$. Now since $z^1 - z^0 = O(h^3)$ in Z^{s_1} , we have $r_3(z^1) - r_3(z^0) = O(h^3)$ in Z^{s_0} . Thus the $O(h^3)$ part cancels, and we conclude that $z_t^1 = F_h(z^1) + O(h^4|\log h|)$ in L_h^2 . The two components of this equation give (6.3) for $p < 4$. The last assertion follows from combining this with (6.2). \square

Proof of (6.27). We need to assess the difference between

$$(7.7) \quad \sum \nabla G_h^\pi(\tilde{x}_j - \tilde{x}_\ell) \cdot \tilde{N}_\ell [(\tilde{n}_\ell \cdot \tilde{n}_j)\tilde{w}_\ell - \tilde{w}_j] h^2$$

and the same where the computed tilde quantities are replaced by the quantities without tildes. To do this we will consider various separate differences by adding and subtracting. (All sums are over $\ell \in I$.) We note first that under the hypothesis (6.6) we have, using Lemmas 6.3 and 6.4

$$(7.8) \quad |\delta n|_{L_h^\infty} \leq Ch^{-1}|\delta n|_{L_h^2} \leq Ch^{-2}|\delta n|_{H_h^{-1}} \leq Ch^{-2}|\delta x|_{L_h^2} \leq Ch^{-2}h^3 = Ch,$$

and similarly for w, N .

We begin with the sum

$$(7.9) \quad \sum \nabla G_h^\pi(x_j - x_\ell) \cdot \tilde{N}_\ell [(\tilde{n}_\ell \cdot \tilde{n}_j)\tilde{w}_\ell - \tilde{w}_j] h^2$$

and consider several differences which, when added to the above, will result in the corresponding sum with no tildes. The first such difference will be the replacement of \tilde{N}_ℓ by N_ℓ . We split this into two terms,

$$(7.10) \quad \sum \nabla G_h^\pi(x_j - x_\ell) \cdot (\delta N_\ell) [(n_\ell \cdot n_j)w_\ell - w_j] h^2,$$

$$(7.11) \quad \sum \nabla G_h^\pi(x_j - x_\ell) \cdot (\delta N_\ell) [\delta((n_\ell \cdot n_j)w_\ell) - \delta w_j] h^2.$$

We view (7.10) as the action on δN of the kernel ∇G_h^π times $(n_\ell \cdot n_j)w_\ell - w_j$. The latter factor is the restriction of a smooth function vanishing on the diagonal, except for a small error, according to the last statement in Lemma 6.2. We ignore the error, since it can be handled as below for (7.11). By Theorem 5.1 the resulting operator has order -1 on L_h^2 , and according to the remark before Lemma 6.3 it is bounded from H_h^{-1} to L_h^2 . Thus the sum (7.10) is bounded in L_h^2 by $C|\delta N|_{H_h^{-1}} \leq C|\delta x|_{L_h^2}$. Now for (7.11), the quantity in brackets is uniformly $O(h)$, according to (7.8) and the analogue for w . We can use the boundedness of ∇G_h^π on L_h^2 , again from Theorem

5.1, to estimate this term by $Ch|\delta N|_{L_h^2} \leq C|\delta N|_{H_h^{-1}} \leq C|\delta x|_{L_h^2}$. Next, to replace \tilde{n}_ℓ by n_ℓ , we consider the difference

$$(7.12) \quad \sum \nabla G_h^\pi(x_j - x_\ell) \cdot N_\ell [\tilde{w}_\ell(\delta n_\ell)] \cdot \tilde{n}_j h^2.$$

Now the operator $\nabla G_h^\pi \cdot N(\alpha_\ell)$ is of order -1 by Theorem 5.1, where $N(\alpha_\ell)$ is the exact normal. Since $N_\ell - N(\alpha_\ell) = O(h^3)$ and ∇G_h^π has order 0, it follows that $\nabla G_h^\pi \cdot N_\ell$ is also of order -1 . Using this fact and Lemmas 6.3 and 6.4, we can estimate (7.12) by $C|\tilde{w}(\delta n)|_{H_h^{-1}} \leq C|\delta n|_{H_h^{-1}} \leq C|\delta x|_{L_h^2}$.

We have now replaced (7.9) with

$$(7.13) \quad \sum \nabla G_h^\pi(x_j - x_\ell) \cdot N_\ell [(n_\ell \cdot \tilde{n}_j)\tilde{w}_\ell - \tilde{w}_j] h^2.$$

If we replace $\tilde{w}_\ell, \tilde{w}_j$ with w_ℓ, w_j , the resulting difference is the first term on the right in (6.27) plus

$$(7.14) \quad (\delta n_j) \cdot \sum \nabla G_h^\pi(x_j - x_\ell) \cdot N_\ell n_\ell(\delta w_\ell)h^2.$$

Since δn_j is uniformly $O(h)$, the last is bounded in L_h^2 by $Ch|\delta w|_{L_h^2}$. Then if we replace \tilde{n}_j by n_j , the difference is

$$(7.15) \quad (\delta n_j) \cdot \sum w_\ell n_\ell \nabla G_h^\pi(x_j - x_\ell) \cdot N_\ell h^2.$$

In the sum above, we can replace w_ℓ with $\phi_n(\alpha_\ell)$, etc., using Lemma 6.2 with small error. The resulting sum is then within $O(h)$ of the integral term in (6.27), according to Theorem 3.7. The term from the quadrature error is bounded in L_h^2 by $Ch|\delta n|_{L_h^2} \leq C|\delta x|_{L_h^2}$. We have now replaced the sum (7.9) with the corresponding sum without tildes, and obtained the two principal terms in (6.27).

Next we consider the difference which results from replacing $\tilde{x}_j, \tilde{x}_\ell$ with x_j, x_ℓ in the sum

$$(7.16) \quad \sum \nabla G_h^\pi(\tilde{x}_j - \tilde{x}_\ell) \cdot N_\ell [(n_\ell \cdot n_j)w_\ell - w_j] h^2.$$

The difference is a similar sum with $\delta \nabla G_h^\pi$ instead of ∇G_h^π . We write $\delta \nabla G_h^\pi = R_2(\alpha_j, \alpha_\ell) \cdot (\delta x_j - \delta x_\ell)$, where R_2 denotes an average of second derivatives of G_h^π along the line from $x_j - x_\ell$ to $\tilde{x}_j - \tilde{x}_\ell$. Since the bracket term vanishes on the diagonal, Theorem 5.1 tells us that the δx_ℓ part of the error is bounded in L_h^2 by $C|\delta x|_{L_h^2}$. For the second part, we factor δx_j out of the sum; the remaining sum is bounded, uniformly in j and h , according to Lemma 5.4. Thus the second part of the error has the same bound as the first.

We are now left with the difference

$$(7.17) \quad \sum \delta \nabla G_h^\pi \cdot \delta [N_\ell((n_\ell \cdot n_j)w_\ell - w_j)]h^2.$$

By considering cases we can see that this is of type $B(\delta x)$. From $\delta \nabla G_h^\pi$ we have R_2 times a factor of δx_j or δx_ℓ , and each term in the second factor has at least one difference in either j or ℓ . We discuss two specific terms. For the term

$$(7.18) \quad \sum R_2 \cdot \tilde{N}_\ell(\delta x_j)(\delta w_j)h^2 = (\delta x_j)(\delta w_j) \sum R_2 \cdot \tilde{N}_\ell h^2$$

we note that $|\tilde{N}_\ell|$ is uniformly bounded, and δw_j is uniformly $O(h)$. The last sum is $O(h^{-1})$, uniformly in j ; this can be seen from the pointwise estimates (2.4) for

$D^m G_h$. Thus the term has the form δx_j times a uniformly bounded function of j . Next we consider the term

$$(7.19) \quad \sum R_2 \cdot \tilde{N}_\ell(\delta x_j)(\delta n_\ell) \tilde{w}_\ell h^2.$$

We can estimate $|(\delta n) \tilde{w}|_{L_h^2}$ by Ch^2 . Then from Theorem 5.1, hR_2 is a bounded operator on L_h^2 , so that the sum omitting the δx_j factor is $O(h)$ in L_h^2 , and therefore $O(1)$ in L_h^∞ . This is then multiplied by δx_j , and the resulting term is $B(\delta x)$. The other terms can be treated by the same methods. \square

Proof of (6.28). We have to find the difference between the sum

$$(7.20) \quad - \sum D_{h,k} G_h^\pi(\tilde{x}_j - \tilde{x}_\ell) \tilde{X}_{k\ell}^* \cdot \tilde{n}_j \tilde{w}_\ell |\tilde{N}_\ell| h^2$$

and the corresponding sum without tildes. We have written out $\nabla_h^T G_h^\pi$, recalling (1.23), with a sum over $k = 1, 2$ implicit. We begin with the sum

$$(7.21) \quad - \sum D_{h,k} G_h^\pi(x_j - x_\ell) \tilde{X}_{k\ell}^* \cdot (\tilde{n}_j - \tilde{n}_\ell) \tilde{w}_\ell |\tilde{N}_\ell| h^2$$

and add differences successively to remove the tildes. We have inserted $-\tilde{n}_\ell$; this does not affect the sum, since $\tilde{n}_\ell \perp \tilde{X}_{k\ell}^*$. We first replace \tilde{n}_j with n_j , resulting in the difference, after a summation by parts,

$$(7.22) \quad -(\delta n_j) \cdot \sum G_h^\pi(x_j - x_\ell) D_{h,k}^* [X_{k\ell}^* w_\ell |N_\ell|] h^2$$

plus a remainder. The remainder has $\delta(X_{k\ell}^* w_\ell |N_\ell|)$, which is $O(h^2)$ in L_h^2 , acted on by $D_{h,k} G_h^\pi$. Since G_h^π is an operator of order -1 on L_h^2 , by Theorem 5.1, $D_{h,k} G_h^\pi$ is bounded, so that the image is $O(h^2)$ in L_h^2 and thus $O(h)$ in L_h^∞ . This is multiplied by δn_j , which is bounded in L_h^2 by $h^{-1} |\delta x|_{L_h^2}$, so that remainder term is of type $B(\delta x)$. As for the main term (7.22), the sum on the right is close to the integral in (6.28), after replacing w_ℓ by $\phi_n(\alpha_\ell)$ etc., with $O(h)$ quadrature error. This last error gives a term bounded by $h |\delta n|_{L_h^2}$ or $|\delta x|_{L_h^2}$.

Next we replace \tilde{n}_ℓ by n_ℓ . The difference is

$$(7.23) \quad \sum D_{h,k} G_h^\pi(x_j - x_\ell) X_{k\ell}^* \cdot (\delta n_\ell) w_\ell |N_\ell| h^2$$

plus a remainder again with $\delta(X_{k\ell}^* w_\ell |N_\ell|)$. As before, the remainder is $B(\delta x)$. We can substitute in (7.23) for δn from (6.12) and obtain the second term on the right in (6.28), up to a remainder which is $B(\delta x)$.

We now have reduced (7.20) to

$$(7.24) \quad - \sum D_{h,k} G_h^\pi(x_j - x_\ell) \tilde{X}_{k\ell}^* \cdot (n_j - n_\ell) \tilde{w}_\ell |\tilde{N}_\ell| h^2.$$

Now since $n_j - n_\ell$ vanishes at $j = \ell$, Theorem 5.2 tells us that the operator with kernel $(n_j - n_\ell) D_{h,k} G_h^\pi$ gains a derivative. Thus, to replace $\tilde{X}_{k\ell}^* |\tilde{N}_\ell|$, we estimate $\tilde{w} \delta(X_k^* |N|)$ in H_h^{-1} by $|\delta x|_{L_h^2}$. The corresponding sum is then bounded by $|\delta x|_{L_h^2}$. To finish with (7.20), we replace \tilde{w}_ℓ with w_ℓ , obtaining as the difference the first term on the right of (6.28).

Next we consider the difference

$$(7.25) \quad \begin{aligned} \sum \delta [D_{h,k} G_h^\pi(x_j - x_\ell)] X_{k\ell}^* \cdot n_j w_\ell |N_\ell| h^2 \\ = \sum [\delta G_h^\pi(x_j - x_\ell)] \cdot n_j D_{h,k}^* [X_{k\ell}^* w_\ell |N_\ell|] h^2. \end{aligned}$$

We write δG_h^π as $R_1(\alpha_j, \alpha_\ell) \cdot (\delta x_j - \delta x_\ell)$, where R_1 is an average of DG_h^π from $x_j - x_\ell$ to $\tilde{x}_j - \tilde{x}_\ell$. For the δx_ℓ part, we conclude from the boundedness of DG_h^π on

L_h^2 that the sum is bounded by $|\delta x|_{L_h^2}$. For the second part, we bring δx_j outside the sum. The remaining sum is uniformly bounded according to Lemma 5.4, and this term is $B(\delta x)$. We are left with more nonlinear terms, which can be handled as at the end of (6.27), after summing by parts to remove $D_{h,k}$ from G_h^π as above. \square

Proof of (6.29). The difference has the form

$$(7.26) \quad \delta(n \cdot \Sigma) = (\delta n) \cdot \Sigma + n \cdot \delta \Sigma + (\delta n) \cdot (\delta \Sigma)$$

Since δn_j is uniformly $O(h)$, by (6.6), it will be evident that the last term can be neglected after we have treated the second term. The sums in the first term are within $O(h)$ of the corresponding integrals, according to Theorem 3.7. (We use summation by parts.) The resulting error term is $B(h\delta n) = B(\delta x)$. The integrals can be converted to the integral in (6.29) by reversing the steps which led to (1.7). Now our task is to evaluate the second term in (7.26).

We treat the first sum in (6.29). As before, we begin with

$$(7.27) \quad n_j \cdot \sum [D_h G_h^\pi, \tilde{X}]_\ell \times (\tilde{\nabla}_h^T \tilde{\phi}_\ell - \tilde{\nabla}_h^T \tilde{\phi}_j) h^2,$$

where $G_h^\pi = G_h^\pi(x_j - x_\ell)$ and $\tilde{\nabla}_h^T f = \sum_{k=1,2} (D_{h,k} f) \tilde{X}_k^*$. We remove the tildes in steps; we first replace $\tilde{\nabla}_h^T \tilde{\phi}_\ell$ with $\nabla_h^T \phi_\ell$. The difference is

$$(7.28) \quad n_j \cdot \sum [D_h G_h^\pi, X]_\ell \times \delta(\nabla_h^T \phi_\ell) h^2$$

plus a remainder with products of δ 's. This remainder is $B(\delta x)$; to see this, we note that $D_h G_h^\pi$ is a bounded operator on L_h^2 and products such as $(\delta X_{1\ell})(D_{h,2} \delta \phi_\ell)$ are bounded in L_h^2 by $|\delta x|_{L_h^2}$, using (6.6). In (7.28) we can substitute for $\delta(\nabla_h^T \phi_\ell)$ from (6.14), obtaining, up to a negligible remainder,

$$(7.29) \quad \sum n_j \cdot [D_h G_h^\pi, X]_\ell \times \nabla_h^T (\delta \phi_\ell - \nabla_h^T \phi_\ell \cdot \delta x_\ell) h^2 \\ + \sum ([D_h G_h^\pi, X]_\ell \times n_\ell) \cdot n_j (\nabla_h^T (n_\ell \cdot \delta x_\ell) \cdot \nabla_h^T \phi_\ell) h^2.$$

In the first sum we substitute $n_j = n_\ell + (n_j - n_\ell)$ and split the sum into two parts. The n_ℓ -part can be converted to the first term on the right in (6.29) using a vector identity as in (1.6). For the remaining part in the first sum of (7.29), we have a smooth factor which vanishes at $\ell = j$, and we can use Theorem 5.2 to show that the sum is $B(\delta x) + B(\delta \phi)$. As for the second sum in (7.29), we note that the cross product is tangential at x_ℓ , so that the scalar product with n_j is zero when $\ell = j$. Thus we can use Theorem 5.2 again to bound this term by $|\delta x|_{L_h^2}$.

Next we replace $\tilde{\nabla}_h^T \tilde{\phi}_j$ in (7.27) by $\nabla_h^T \phi_j$. The difference is

$$(7.30) \quad n_j \cdot \delta(\nabla_h^T \phi_j) \times \sum [D_h G_h^\pi, X]_\ell h^2,$$

except for an error nonlinear in the δ 's which is again negligible. The sum in (7.30) is within $O(h)$ of an integral which is zero; see (1.5), (1.8), (1.28). The term with the quadrature error is of order $h|\delta \nabla_h^T \phi|_{L_h^2}$, which in view of (6.14) is $B(\delta \phi) + B(\delta x)$. We have now reduced (7.27) to

$$(7.31) \quad n_j \cdot \sum [D_h G_h^\pi, \tilde{X}]_\ell \times (\nabla_h^T \phi_\ell - \nabla_h^T \phi_j) h^2.$$

The last factor vanishes when $\ell = j$, and we can therefore use Theorem 5.2 to replace \tilde{X}_ℓ with X_ℓ , with a difference $B(\delta x)$, thus completing the treatment of (7.27).

The most important remaining term from the first sum on the left in (6.29) is

$$(7.32) \quad n_j \cdot \sum [\delta(D_h G_h^\pi), X]_\ell \times (\nabla_h^T \phi_\ell - \nabla_h^T \phi_j) h^2.$$

This can be treated similarly to the corresponding term in (6.28). The other terms are nonlinear and can be handled like earlier cases. The variation of the second sum can be treated by techniques as for (6.27), but more simply. We need to use the fact that $\nabla_h^T \phi_j$ is multiplied by a discretization of an integral which is zero by (1.5). \square

Proof of Lemma 6.7. The operator $\tilde{\mathcal{K}}_h$ differs from \mathcal{K}_h by an operator which is $O(h)$. This can be shown by estimates related to (6.27), (6.28) but simpler. By the remarks in the proof of Lemma 6.1, $2\tilde{\mathcal{K}}_h$ then has spectral radius less than one, and it follows that the discrete integral equation can be solved by simple iteration. \square

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DEPARTMENT OF MATHEMATICS, DUKE UNIVERSITY, DURHAM, NC 27708-0320
E-mail address: beale@math.duke.edu