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THE BASIS SPLINE METHOD AND ASSOCIATED TECHNIQUES

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THE BASIS SPLINE METHOD
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ABSTRACT

We outline the Basis Spline and Collocation methods for the solution of Partial Differential Equations. Particular attention is paid to the theory of errors, and the handling of non-self-adjoint problems which are generated by the collocation method. We discuss applications to Poisson's equation, the Dirac equation, and the calculation of bound and continuum states of atomic and nuclear systems.

*We can forgive a man for making a useful thing
as long as he does not admire it.*

*The only excuse for making a useless thing
is that one admires it intensely.*

All art is quite useless.

OSCAR WILDE (*The Picture of Dorian Gray*)

1. THE BASIS SPLINE AND COLLOCATION METHODS

1.1 Basis Splines and their Generation

Splines of order \mathcal{N} are functions $S^{\mathcal{N}}(x)$ of a single real variable belonging to the class $C^{\mathcal{N}-2}$ with continuous $(\mathcal{N} - 2)^{\text{th}}$ derivatives. Each spline is associated with a set of points $\{x_k\}$, called knots; we take the knots to be distinct and ordered, $x_k < x_{k+1}$. Between each pair of knots, the spline is a polynomial of degree $\mathcal{N} - 1$ (the order refers to the number of coefficients); at each knot, the function and derivatives up to the $(\mathcal{N} - 2)^{\text{th}}$ are continuous. The $(\mathcal{N} - 1)^{\text{th}}$ derivative is bounded but discontinuous. We shall consider only orders $\mathcal{N} \geq 3$, though piecewise linear or tent functions ($\mathcal{N} = 2$) were useful at an earlier stage in development of numerical analysis, particularly as the simplest implementation of the finite element method.

Splines have long been used for curve fitting, but the introduction of basis splines converted the concept into a power technique. Given a set of knots $\{x_k\}$, the basis splines of order \mathcal{N} are a set of functions $B_k^{\mathcal{N}}(x)$ such that any spline $S^{\mathcal{N}}(x)$ is identically a linear superposition

$$S(x) \equiv \sum_k a_k B_k^{\mathcal{N}}(x). \quad (1)$$

It is easy to see that $B_k^{\mathcal{N}}(x)$ is uniquely defined by the condition that it is zero outside the range of $\mathcal{N} + 1$ consecutive knots $x_k, x_{k+1}, \dots, x_{k+\mathcal{N}}$. Such a function of order $\mathcal{N} = 3$ is illustrated in Fig. 1. At either end of the range of knots, the basis splines can be modified to incorporate boundary conditions. As an example, Fig. 2 shows how a set of splines can be fitted together to represent functions

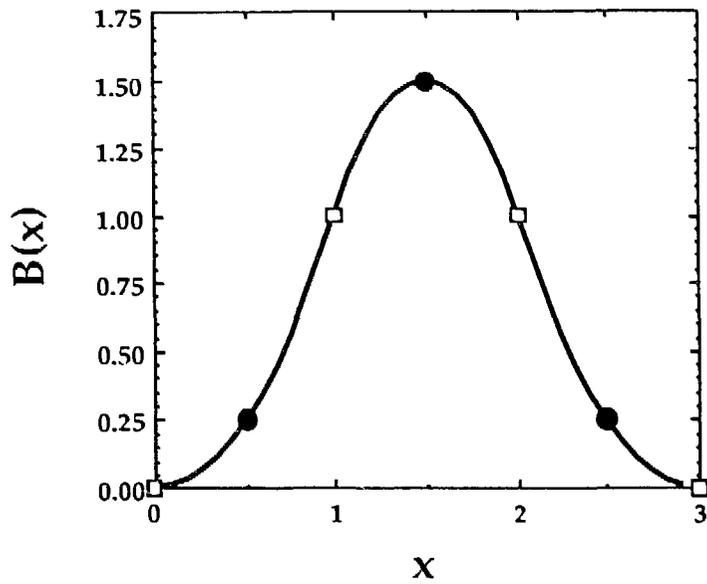


Fig. 1. Basis spline of order $\mathcal{N} = 3$. The knots are denoted by open squares, and the collocation points by filled circles.

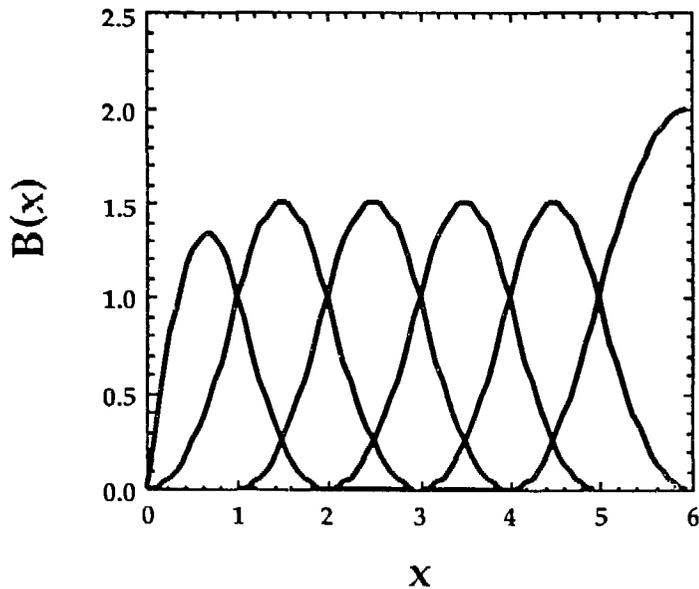


Fig. 2. Basis splines of order 3 satisfying the boundary conditions (2).

satisfying the boundary conditions

$$\psi(x_1) = 0, \quad \psi'(x_N) = 0, \quad (2)$$

where the prime denotes differentiation. Several algorithms are available to construct basis splines from the continuity conditions at the knots, and the boundary conditions at the endpoints ^{1,2,4,5)}, and we refer the reader to the literature rather than pursue this rather technical aspect of the subject here.

Given the basis splines, interpolation is straightforward. A function $\psi(x)$ is approximated by the interpolant $\hat{\psi}$, where

$$\hat{\psi}(x) = \sum_{k=1}^N \psi^k B_k(x), \quad (3)$$

and the ψ^k are determined if $\hat{\psi}(x) \equiv \psi(x)$ at a set of N data, or *collocation*, points $\{\xi_\alpha\}$. We have only to solve

$$\sum_{k=1}^N B_{\alpha k} \psi^k = \psi_\alpha, \quad (4)$$

where $B_{\alpha k} = B_k(\xi_\alpha)$ and $\psi_\alpha = \psi(\xi_\alpha)$; the order \mathcal{N} is omitted for simplicity. It is necessary and sufficient that the matrix \mathbf{B} be non-singular: this will always be the case if we limit our considerations to odd orders, and choose the collocation points halfway between the knots. Further, as is clearly seen in Fig. 1, the elements of \mathbf{B} are positive and largest on the diagonal, implying that the inversion of (4) is very stable. It is convenient to have a notation for the inverse of \mathbf{B} : we write the elements as $B^{k\alpha}$ so that

$$\sum_{k=1}^N B^{k\alpha} \hat{\psi}^k = \psi^k. \quad (5)$$

Formulae for derivatives and integrals are readily derived from (3)-(5) ⁴⁾.

1.2 Collocation Methods

The collocation method for solution of an operator equation, formally written as

$$L[\psi] = 0 , \quad (6)$$

is intimately related to the interpolation procedure of (3) and (4). We obtain N equations for the unknowns $\{\psi^k\}$ by requiring that

$$L[\sum \psi^k B_k] = 0 \text{ at } x = \xi_\alpha . \quad (7)$$

Though the method is perfectly applicable to non-linear problems, we are mostly concerned with linear operators L , in which case (7) becomes

$$\sum_{k=1}^N \psi^k L[B_k]_{x=\xi_\alpha} = 0 . \quad (8)$$

If we use (4) and (5) to eliminate the coefficients $\{\psi^k\}$ in favour of the values of the solution $\{\psi^k\}$ at the collocation points,(8) is replaced by

$$\sum_{\alpha=1}^N L_{\beta\alpha} \psi_\alpha = 0 , \quad (9)$$

where

$$L_{\beta\alpha} = \sum_{k=1}^N B^{k\alpha} L[B_k]_{x=\xi_\beta} = 0 . \quad (10)$$

As a simple example, consider the non-relativistic Schrödinger equation in one dimension,

$$(T + V)\psi = \left[-\frac{1}{2} \frac{d^2}{dx^2} + V(x) \right] = 0 , \quad (11)$$

where V is a local potential. An agreeable feature of the method is that expressions such as $V\psi$ are replaced by $V_\alpha\psi_\alpha$, where $V_\alpha = V(\xi_\alpha)$. In other words, local operators come to be represented simply as diagonal matrices of their values at the collocation points. Non-local operators, notably the kinetic energy, appear complicated at first sight. In summary, (11) is replaced by

$$\sum_{\beta=1}^N (T_{\alpha\beta} + V_\alpha\delta_{\alpha\beta})\psi_\beta = E\psi_\alpha, \quad (12)$$

where

$$T_{\alpha\beta} = -\frac{1}{2} \sum_{k=1}^N B''_{\alpha k} B^{k\beta},$$

$$B''_{\alpha k} = \left[\frac{d^2 B_k}{dx^2} \right]_{x=\xi_\alpha}. \quad (13)$$

We shall see in Section 2 that the analysis of (6)-(13) is readily extended to problems in two and three dimensions.

1.3 Completeness and Convergence

Given a formal interpolation procedure, such as that implied by (3)- (5), the issue of completeness refers to how well the interpolant $\hat{\psi}(x)$ represents $\psi(x)$ at points other than the exactly fit points $\{\xi_\alpha\}$. In other words, how does the error

$$\mathcal{E}(x) = |\psi(x) - \hat{\psi}(x)| \quad (14)$$

behave globally? A simple estimate is obtained from the Dirichlet functions $B_k(x)$, which arise when $\hat{\psi}$ is expressed directly in terms of $\{\psi_\alpha\}$. From (3)-(5), we find that

$$\hat{\psi}(x) = \sum_{k=1}^N \psi_\alpha \hat{B}_\alpha(x),$$

$$\hat{B}_\alpha(x) = \sum_{k=1}^N B^{k\alpha} B_k(x). \quad (15)$$

A typical Dirichlet function is shown in Fig. 3. It is evident that $\hat{B}_\alpha(\xi_\beta) = \delta_{\alpha\beta}$ by construction, but at other points, \hat{B}_α is non-zero and oscillating in sign. The values of $|\hat{B}_\alpha|$ at successive turning points ξ'_β fall off rapidly, in fact approximately as

$$0.3 \exp \left[-\frac{(\xi_\alpha - \xi'_\beta)^2}{2N\Delta^2} \right],$$

for knots with a uniform spacing Δ ⁴). At the first minimum, however, $\hat{B}_\alpha \simeq -0.3$.

Thus the maximum of the error function (14) is estimated to be

$$\mathcal{E}_{\max} \simeq 0.3 \max_{\alpha} |\psi_{\alpha+1} - \psi_{\alpha}|. \quad (16)$$

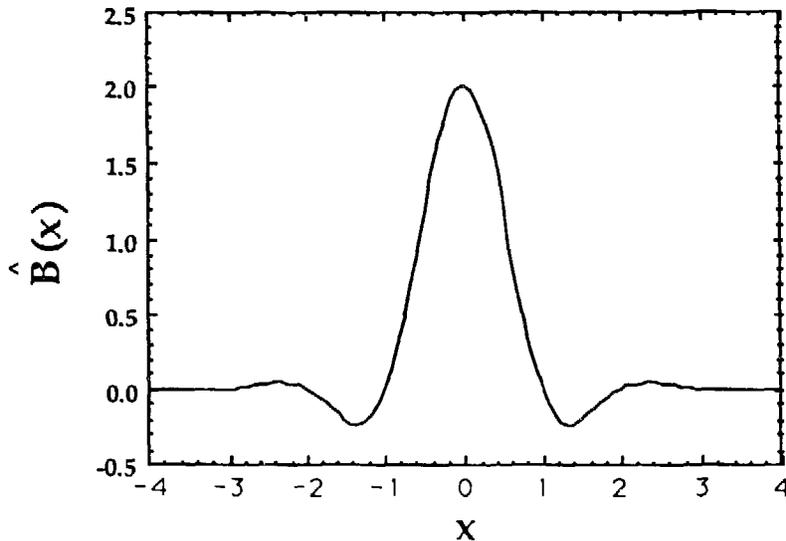


Fig. 3. Dirichlet function of order 3: $\hat{B}(x)$ is defined in (15).

A large error is encountered if ψ has a discontinuity, as seen in Fig. 4, which depicts the result of trying to fit a step function. However, in virtue of the rapid

rate of falling off of $\hat{B}_\alpha(x)$ with $|x - \xi_\alpha|$, the overshooting oscillations in the fit also die off rapidly with distance from the discontinuity. This contrasts with the notorious behaviour of Fourier or orthogonal polynomial interpolation.

When splines are used to fit smooth functions (of class C^M , $M > 1$, say), the solutions to operator problems usually converge uniformly as the number of points is increased. Uniformity implies, in quantum mechanical problems such as (11), that the wavefunction converges at the same rate as the eigenvalue. A further point, of great practical significance, is that the rate of convergence improves as the order of the splines increases: usually $\mathcal{E} \sim \Delta^{-\mathcal{N}+1}$.

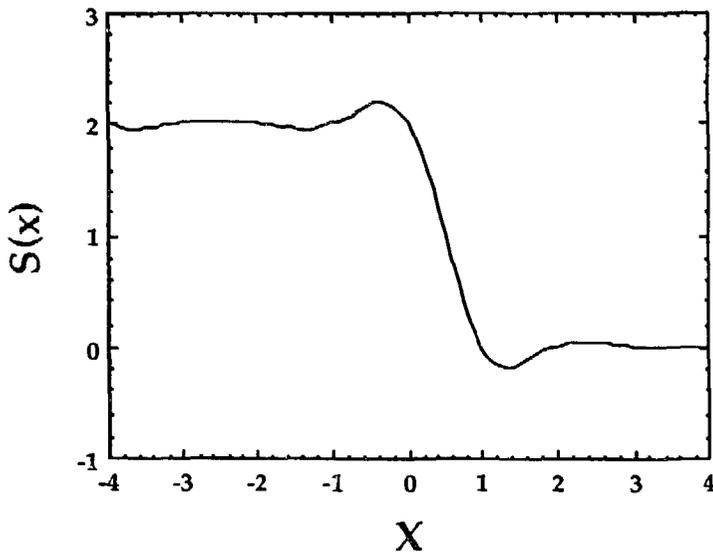


Fig. 4. Result of fitting a step function $S(x)$ with splines of order 3.

This is illustrated by Fig. 5 which shows the errors in the lowest eigenvalue of (11), where V is chosen to be a Morse potential⁴⁾. Usually $\mathcal{N} = 7$ is adequate for practical purposes. Though spline interpolation remains stable for any order,

a trend of diminishing returns is usually observed for $\mathcal{N} > 7$; for increasing \mathcal{N} more splines may be needed to accommodate the boundary conditions instead of representing the solution.

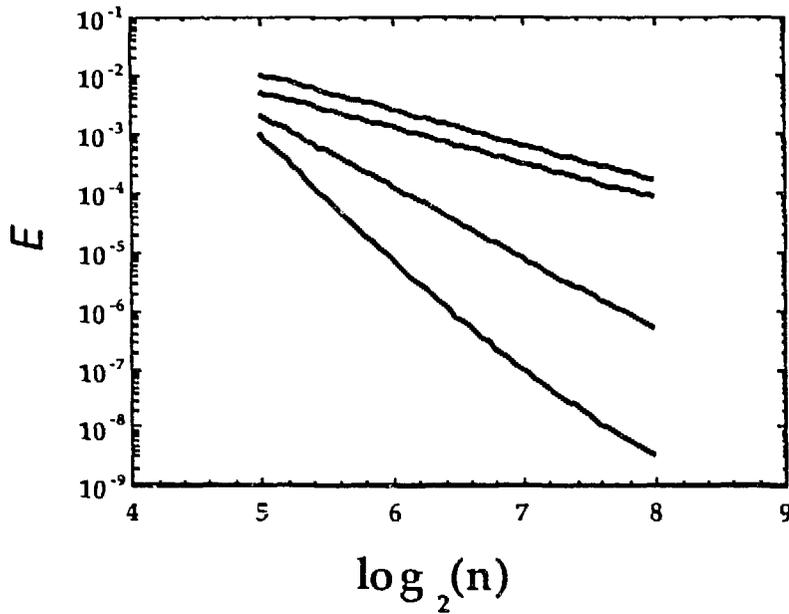


Fig. 5. Errors in the lowest eigenvalue of a Morse potential *vs.* the number of grid points n for different discretization algorithms. Reading from the top down, the curves refer to the 3-point finite difference method, and the basis spline-collocation method with splines of orders 3, 5 and 7 respectively. The model is described in more detail in Ref. 4).

1.4 Techniques for Non-Self Adjoint Problems

The most general collocation-variational method for the linear operator equation $L\psi = 0$ is obtained by expanding ψ in a righthand basis u_k , and projecting the equation onto a lefthand basis v_α ,

$$\sum_k (v_\alpha, Lu_k) \psi^k = 0. \quad (17)$$

The collocation method results from the choice $v_\alpha = \delta(x - \xi_\alpha)$, and the self-

adjoint variational method from the choice $v_\alpha = u_\alpha$. For a general choice of v_α , including that of the collocation method, (17) is not self adjoint. Though problems which are not self adjoint are not usually emphasised in textbooks, they pose no great difficulties. In some branches of physics, such as transport phenomena and quantum optics, non-self-adjoint formulations may be more natural.

We are interested in the stationary eigenvalue problem of quantum mechanics, $L = H - E$, for which the collocation procedure results in a non-self-adjoint matrix problem,

$$\begin{aligned} \mathbf{H}\psi^{(\lambda)} &= \epsilon^{(\lambda)}\psi^{(\lambda)}, \\ \mathbf{H}^\dagger\phi^{(\lambda)} &= \epsilon^{(\lambda)}\phi^{(\lambda)}, \end{aligned} \tag{18}$$

where the right and lefthand eigenvectors are biorthogonal $\phi_\lambda^\dagger\psi_\mu = \delta_{\lambda\mu}$. If we define a matrix Ψ whose elements are $\Psi_{\beta\lambda} = \psi_\beta^{(\lambda)}$, a similar matrix Φ , and a diagonal matrix of the eigenvalues ϵ , (18) becomes

$$\mathbf{H}\Psi = \Psi\epsilon, \quad \mathbf{H}^\dagger\Phi = \Phi\epsilon. \tag{19}$$

The two equations (19) are only consistent if

$$\Psi^{-1} = \Phi^\dagger, \quad \Phi^{-1} = \Psi^\dagger. \tag{20}$$

It is necessary and sufficient that the eigenvectors be linearly independent. From (19) and (20) the reconstruction of the matrix from its eigenvectors is given by

$$\mathbf{H} = \Psi\epsilon\Psi^{-1} = \Psi\epsilon\Phi^\dagger. \tag{21}$$

The significance of (21) is that H may be factored into a self-adjoint operator \hat{H} , and a positive, definitive self adjoint operator S^{-1} ,

$$\mathbf{H} = S^{-1}\hat{H}. \quad (22)$$

where

$$\hat{H} = \Phi\epsilon\Phi^\dagger, \quad S = \Psi\Psi^\dagger. \quad (23)$$

If the eigenvectors are linearly independent, S is non-singular and can be interpreted as an overlap matrix between a set of linearly independent basis functions.

The factorization (23) converts (19) into a *generalized eigenvalue problem*,

$$\mathbf{H}\Psi = S\Psi\epsilon. \quad (24)$$

The factorization (22) is necessary and sufficient for \mathbf{H} to possess a real spectrum.

It is instructive to pursue the physical interpretation of the lefthand eigenvectors. Given (18), the only consistent prescription for the expectation value of a local operator $a(x)$ in the eigenstate λ is

$$\langle a \rangle = \phi^{(\lambda)\dagger} \mathbf{a} \psi^{(\lambda)} = \sum_{\alpha} \phi_{\alpha}^{(\lambda)*} a(\xi_{\alpha}) \psi_{\alpha}^{(\lambda)}. \quad (25)$$

This agrees intuitively with the usual formula of wave mechanics,

$$\langle a \rangle = \int dx \psi^*(x) a(x) \psi(x),$$

if we identify

$$\psi_{\alpha}^{(\lambda)} \longrightarrow \psi(\xi_{\alpha}), \quad \phi_{\alpha}^{(\lambda)} \longrightarrow W_{\alpha} \phi(\xi_{\alpha}), \quad (26)$$

and $\{W_\alpha\}$ are the quadrature weights associated with the points $\{\xi_\alpha\}$. The identification (26) suffers from the drawback that the weights have a dependence on λ and do not coincide identically with the conventional definition of numerical analysis,

$$W_\alpha = \int dx \hat{B}(x) .$$

Nonetheless (26) can sometimes be used to good effect, as we shall see in Sections 1.5 and 2.2.

1.5 Representation Theory

The concept of a *faithful* representation of a differential operator is taken over from the mathematical literature ¹⁾. For our purposes, it means that the representation faithfully simulates the familiar intuitive properties of the differential calculus. No approximation can reproduce all properties exactly, but we can base our development on the following choice. Given the operator $D = d/dx$, we require that its matrix representation \mathbf{D} satisfies a subset of identities

$$\mathbf{D}\chi_M = \chi_{M-1} , \tag{27}$$

analogous to those for differentiating the monomials

$$\chi_M(x) = \frac{x^M}{M!} . \tag{28}$$

Insofar as the basis splines belong to the class $C^{\mathcal{N}-2}$, (27) holds identically for $M \leq \mathcal{N} - 2$. In general, the identity is modified near the boundaries, since

the polynomial representation must be constrained to accommodate the boundary conditions.

We remarked above that differential operators in the basis-spline-collocation representation had a rather recondite appearance. However, when the numerical presentation is examined, it becomes obvious that the operators have the qualitative and intuitive structure expected from elementary finite difference considerations. An example will make the point more clearly. If the second derivative operator is constructed as in (13), with periodic boundary conditions on a mesh with unit spacing and spline order $\mathcal{N} = 3$, the elements of the resulting matrix are given by

$$D_{\alpha, \alpha+\mu}^{(2)} = (\dots, -0.0049, 0.0286, -0.1665, 0.9705, -1.657, \\ 0.9705, -0.1665, 0.0286, \dots) .$$

It is easy to see that the sum across a row is zero to good accuracy, and that the pattern of elements resembles the finite difference representation

$$D_{\alpha, \alpha+\mu}^{(2)} = (\dots, 0, 1, -2, 1, 0, \dots) .$$

These properties of $D^{(2)}$ make it a faithful representation of d^2/dx^2 .

To develop these ideas more quantitatively, consider the simplest representation of a derivative, by a single backward difference,

$$\mathbf{D} = \begin{bmatrix} 1 & 0 & 0 & 0 & \cdots \\ -1 & 1 & 0 & 0 & \cdots \\ 0 & -1 & 1 & 0 & \cdots \\ & & & \cdots & 1 & 0 \\ & & & & \cdots & -1 & 1 \end{bmatrix} . \quad (29)$$

This representation satisfies an identity of the form (27),

$$\mathbf{D}\chi_0 = \mathbf{e} , \quad (30)$$

where $\chi_{0\alpha} = 1 \forall \alpha$ and $e_\alpha = \delta_{\alpha,1}$. In general χ is the eigenvector of the modified operator $\tilde{\mathbf{D}}$ corresponding to a zero eigenvalue, where

$$\tilde{D}_{\alpha\beta} = D_{\alpha\beta} - \delta_{\alpha,1}\delta_{\beta,1} . \quad (31)$$

The accompanying righthand eigenvector ω_0 defines a set of quadrature weights in accordance with the prescription (26),

$$\omega_0^\dagger \mathbf{D} = \mathbf{e}^\dagger , \quad (32)$$

where ω_0 is so normalized that $\omega_{01} = 1$. The significance of (32) is seen by applying both sides to an arbitrary vector ψ ,

$$\omega_0^\dagger \mathbf{D}\psi = \psi_1 , \quad (33)$$

which is the familiar formula for the integral of a derivative. Higher moments are obtained by repeatedly operating on \mathbf{e} with \mathbf{D}^{-1} ,

$$\chi_M = \mathbf{D}^{-M-1} \mathbf{e} . \quad (34)$$

In summary, the formal requirement of fidelity (30) leads to a quadrature formula which is identically inverse to differentiation on the lattice. This, in turn, leads to an analogue of Green's lemma as an identity on the lattice, and finally to exact conservation laws on the lattice ⁴⁾.

2. APPLICATIONS

2.1 Atomic and Nuclear Collision Problems

One of the most powerful techniques for studying atomic and nuclear collisions is the numerical Time-Dependent Hartree-Fock (TDHF) method. This amounts to solving a set of partial differential equations in three spatial dimensions, in addition to time. Most current work is based on cartesian, rather than curvilinear coordinates. For a system with A independent particle orbits, the orbital wavefunctions satisfy

$$\begin{aligned}
 H\psi_K &= i\frac{\partial\psi_K}{\partial t} \quad (K = 1, \dots, A), \\
 H &= T_x + T_y + T_z + V(x, y, z|t),
 \end{aligned}
 \tag{35}$$

where

$$T_x = -\frac{1}{2}\frac{\partial^2}{\partial x^2}, \dots$$

The potential energy is the sum of the self-consistent field \mathcal{V} , and an external time-dependent part U , which in atomic physics would be provided by the nuclear motion. The self-consistent field \mathcal{V} depends on the orbitals through Poisson's equation,

$$\nabla^2 \mathcal{V} = -4\pi \sum_{K=1}^A n_K |\psi_K|^2, \quad (36)$$

where n_K is the occupancy of the K^{th} orbital. Thus the equations are coupled through nonlinear interactions, though the nonlinearity is very weak in atomic physics. The foregoing presentation is rather schematic — the reader is referred to the literature^{6,7,8,9)} for an explanation of the complications arising from spin and the Pauli exclusion principle.

The coupled set (35) and (36) are ideally suited to the basis spline-collocation approach. The procedure of (7) is generalized by expanding the wavefunction in products

$$\psi(x, y, z) = \sum_{ijk} \psi^{ijk} B^i(x) B^j(y) B^k(z). \quad (37)$$

For simplicity of exposition, we assume that the same set of splines is associated with each coordinate. In collocation space, we find that the representation of the Hamiltonian analogous to (12) is given by

$$\begin{aligned} H_{\alpha\beta\gamma, \alpha'\beta'\gamma'} = & T_{\alpha, \alpha'}^x \delta_{\beta, \beta'} \delta_{\gamma, \gamma'} + T_{\beta, \beta'}^y \delta_{\gamma, \gamma'} \delta_{\alpha, \alpha'} + T_{\gamma, \gamma'}^z \delta_{\alpha, \alpha'} \delta_{\beta, \beta'} \\ & + V(\xi_\alpha, \xi_\beta, \xi_\gamma) \delta_{\alpha, \alpha'} \delta_{\beta, \beta'} \delta_{\gamma, \gamma'}, \end{aligned} \quad (38)$$

where $T_{\alpha, \alpha'}^x$ is given by (13).

The equations (35) now have the form

$$i \frac{\partial}{\partial t} \psi = \mathbf{H} \psi, \quad (39)$$

where \mathbf{H} is the sum of block matrices of a rather simple form. Thus algorithms which decompose into canonical operations of the form

$$\mathbf{H}\psi \longrightarrow \psi' , \quad (40)$$

can be implemented efficiently on supercomputers with vector and parallel capabilities. Such an algorithm is used for time propagation. If time is divided into small steps τ ,

$$\psi(t + \tau) = \exp[-i\mathbf{H}(t + \tau/2)]\psi(t) , \quad (41)$$

with an error of order $\mathcal{O}(\tau^3)$. The exponential can be expanded in a power series using only operations of the form (40).

Propagation in time is only one aspect, and probably the simplest, of the complete solution of a collision problem. In the following sections, we treat the other aspects in turn:

- Solution of Poisson's equation (36).
- Construction of initial conditions by solution of the stationary eigenvalue problem.
- Extraction of continuum amplitudes by projection on final states.

2.2 Poisson's Equation

It is convenient to rewrite Poisson's equation (36) as

$$(\epsilon - T_x - T_y - T_z)\phi = 2\pi\rho , \quad (42)$$

where T_x is the kinetic energy operator associated with the x-coordinate, as before, and ϵ is a small positive quantity. This equation is to be solved in a finite domain

Ω , bounded by a closed surface Σ , with the boundary condition that the normal derivative is known on Σ ,

$$\frac{\partial\phi}{\partial n} = g(S), \quad S \in \Sigma. \quad (43)$$

The function $g(S)$ is usually constructed from a multipole expansion. It is important that (42) and (43) be consistent in the sense of satisfying Gauss's theorem for the total charge within Ω ,

$$Q = \int_{\Omega} \rho d\tau = \int_{\Sigma} g dS. \quad (44)$$

To incorporate the boundary condition (43), we transform the source in (42),

$$(\epsilon - T_x - T_y - T_z)\hat{\phi} = 2\pi\hat{\rho} = 2\pi[\rho - g(S)\delta(S)], \quad (45)$$

so that the righthand side integrates to zero over Ω . Introducing a basis spline expansion, (45) can be discretized by the methods of earlier sections,

$$(\epsilon - \mathbf{T}_x - \mathbf{T}_y - \mathbf{T}_z)\hat{\phi} = 2\pi\hat{\rho}, \quad (46)$$

The boundary delta-function $\delta(S)$ is written as a sum of Kronecker deltas with appropriate weights. The old and new solutions, ϕ and $\hat{\phi}$, differ only by a constant in their exact (or continuum) representation. However in their matrix representation on a lattice, the relationship is more recondite. Suppose there exists a pair of left and right eigenvectors corresponding to a zero eigenvalue of $T = T_x + T_y + T_z$,

$$(\epsilon - \mathbf{T})\theta = 0, \quad \tilde{\theta}^\dagger(\epsilon - \mathbf{T}) = 0, \quad (47)$$

Then ϕ and $\hat{\phi}$ differ by a multiple of θ , and (46) has a solution only if

$$\bar{\theta}^\dagger \hat{\rho} = 0 . \quad (48)$$

According to the principles of Section 1.5, in particular (26), the elements of θ are quadrature weights, and (48) is the lattice form of Gauss's theorem. The existence of a zero eigenvalue thus guarantees a well-behaved solution. A zero eigenvalue mandates a zero gradient on the boundary: periodic boundary conditions or $\partial\psi/\partial n = 0$ are acceptable, but $\psi = 0$ is not.

The eigenvalue spectrum of \mathbf{T} is readily constructed from that of \mathbf{T}_x ,

$$\mathbf{T}_x \boldsymbol{\eta}_k = \tau_k \boldsymbol{\eta}_k, \quad \mathbf{T}_x^\dagger \tilde{\boldsymbol{\eta}}_k = \tau_k \tilde{\boldsymbol{\eta}}_k, \quad (49)$$

with the identifications,

$$\tau_0 = 0, \quad , \eta_{0\alpha} = 1, \quad , \tilde{\eta}_{0\alpha} = W_\alpha, . \quad (50)$$

We can transform the source and solution of (45) to the new basis provided by (50),

$$\begin{aligned} \hat{\rho}_{\alpha\beta\gamma} &= \sum_{ijk} \eta_{i\alpha} \eta_{j\beta} \eta_{k\gamma} \hat{\rho}_{[ijk]}, \\ \hat{\phi}_{\alpha\beta\gamma} &= \sum_{ijk} \eta_{i\alpha} \eta_{j\beta} \eta_{k\gamma} \hat{\phi}_{[ijk]} . \end{aligned} \quad (51)$$

In this representation, the solution of (45) is simply,

$$\hat{\phi}_{[ijk]} = (\epsilon - \tau_i - \tau_j - \tau_k)^{-1} \hat{\rho}_{[ijk]} . \quad (52)$$

It follows from (48) and (51) that $\hat{\rho}_{[000]} = 0$. Thus (51) and (52) define the solution within a constant, which can be fixed by invoking the multipole expansion again.

2.3 Bound State Eigenfunctions and Continuum State Amplitudes

As stated above, we require a means of setting up the initial conditions of the scattering problem (35), as expressed in matrix form (39). These usually state that ψ is the stationary ground state satisfying

$$\mathbf{H}\psi_0 = E_0\psi_0, \quad (53)$$

with a similar equation for the adjoint vector ϕ_0 . The matrix \mathbf{H} is usually too large to store explicitly in core, so we seek iterative methods which require only “operator knowledge”, meaning the implicit ability to carry out the canonical operation (40). Such a technique is the *damped relaxation* method, described in detail in a recent paper¹⁰⁾. The ground state eigenvector of the Schrödinger equation is the limit of the iterates $\psi^{(I)}$, generated by

$$\psi^{(K+1)} - \psi^{(K)} = v\mathbf{R}[\mathbf{H} - E^{(I)}], \quad (54)$$

where $E^{(I)} = \psi^{(K)\dagger}\mathbf{H}\psi^{(K)}$, and \mathbf{R} is a relaxation operator, designed to filter out the high-frequency components of $\psi^{(K)}$. A convenient choice for \mathbf{R} is

$$\mathbf{R} = \left(1 + \frac{\mathbf{T}_x}{\mu}\right)^{-1} \left(1 + \frac{\mathbf{T}_y}{\mu}\right)^{-1} \left(1 + \frac{\mathbf{T}_z}{\mu}\right)^{-1}. \quad (55)$$

An extensive theory has been developed on the optimum choice of μ and v to guarantee rapid convergence.

Excited states ψ_m can be computed by enforcing the constraint of orthogonality to lower lying states. Then bound state amplitudes can be extracted from the final state wavefunction $\psi(T)$ by projection,

$$P_m = |\phi_m^\dagger \psi(T)|^2 . \quad (56)$$

Amplitudes may be calculated in a frame moving with one of the nuclei by using the eigenstates of a translated Hamiltonian

$$H' = H - \vec{v} \cdot \vec{p} , \quad (57)$$

where \vec{v} is the nuclear velocity.

Direct calculation of every eigenvector is not practical for continuum amplitudes, so we use another technique, that of the *Gaussian filter*^{11,12)}. Suppose we expand

$$\psi(T) = \int dE \sum_\lambda A_\lambda(E) \Psi_\lambda(E) , \quad (58)$$

where λ distinguishes substates of the same energy. The amplitudes can be picked out of (58) by operating on ψ with the filter

$$F(E, \Delta) = (\sqrt{\pi}\Delta)^{-1/2} \exp \left[\frac{(E - H)^2}{2\Delta^2} \right] . \quad (59)$$

Defining $\theta = F(E, \Delta)\psi(T)$, it is easily shown that for moderately small Δ

$$\sum_\lambda |A_\lambda(E)|^2 \simeq \theta^\dagger \theta . \quad (60)$$

With some refinements, it is possible to extract other information, such as angular distributions.

In more recent work¹²⁾, we do not use the Gaussian (59) as such, but replace the exponential by a rational function

$$\exp(-Z) \longrightarrow \left(1 + \frac{Z}{M} \right)^{-M} ,$$

where the inversion is performed by damped relaxation.

2.4 The Dirac Equation

Discrete representations of the Dirac equation are plagued by the pathology of “fermion doubling”, namely the appearance of high momentum components at low energies. We briefly indicate how this problem is avoided in the basis spline-collocation method ⁴⁾.

It is sufficient to consider the continuum states of a free particle in one dimension. The upper and lower components g, f satisfy

$$\begin{aligned} g - f' &= E g \\ f + g' &= E f . \end{aligned} \tag{61}$$

The pathology arises when (61) is discretized on a uniform mesh with the prescription

$$g'_n \simeq \frac{g_{n+1} - g_{n-1}}{2\Delta x} , \tag{62}$$

manifesting itself in a double valued dispersion relation, as illustrated in Fig. 6.

If by contrast we use forward and backward differences

$$f'_n \simeq \frac{f_{n+1} - f_n}{\Delta x} , \quad g'_n \simeq \frac{g_n - g_{n-1}}{\Delta x} , \tag{63}$$

a single valued relation is recovered.

In the basis spline-collocation method, we generalize this procedure by factorizing the second derivative representation

$$D^{(2)} = D_- D_+ , \tag{64}$$

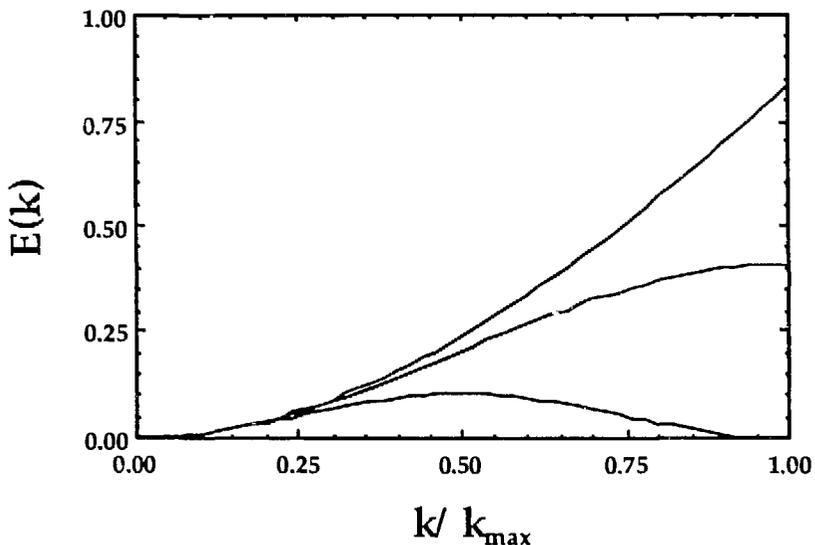


Fig. 6. Energy-momentum dispersion relation $E(k)$ for a free particle obeying the one dimensional Dirac equation. Reading from the top down, the curves refer to the exact continuum result, discretization using (62), and using (63).

and replacing

$$f' \longrightarrow D_+ f, g' \longrightarrow D_- g.$$

This procedure can be justified from fidelity arguments⁴⁾. If $D^{(2)}$ satisfies an identity of the form (30), then (64) is the only factorization leading to operators which satisfy similar identities.

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