

Quantum Mechanics

and the

Finite Element Method

Robert Gilmore

Physics Department, Drexel University, Philadelphia, PA 19104

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Abstract

Schrödinger's equation usually cannot be solved analytically. It is even difficult to solve numerically when the boundary conditions are anything but straightforward. When finite difference schemes come up short, finite element methods are often useful. This is a simple tutorial for the finite element method applied to quantum mechanical problems.

1 Wave Mechanics

The very first formulation of Wave Mechanics by Schrödinger was variational:

$$\delta \int \left\{ \frac{\hbar^2}{2m} \nabla \psi(x)^* \cdot \nabla \psi(x) + \psi^*(x) V(x) \psi(x) - \psi^*(x) E \psi(x) \right\} d^3x = 0 \quad (1)$$

Here $\psi(x)$ is some sort of wavefunction that somehow describes the properties of the particle, $V(x)$ is the potential the particle moves in, and E is the particle energy. The term $\nabla \psi(x)^* \cdot \nabla \psi(x)$ measures the curvature of the wavefunction. In some way it is a surrogate for the (kinetic) energy of the particle. Schrödinger never came to terms with the physical meaning of $\psi(x)$.

From this equation, Schrödinger proceeded to carry out an integration by parts. This resulted in an expression involving a second derivative ($\nabla^2 \psi(x)$) that we now call Schrödinger's equation.

2 Matrix Mechanics

The transformation from Wave Mechanics to Matrix Mechanics is effected by sampling the wavefunction, the potential, and the "kinetic energy" at a (discrete) set of points. We take these points to be in the appropriate configuration space. The wavefunctions and the potential are approximated throughout space in terms of a *basis set* of real functions:

$$\psi^*(x) = \sum_i \phi_i f_i(x) \quad V(x) = \sum_j V_j f_j(x) \quad \psi(x) = \sum_k \psi_k f_k(x) \quad (2)$$

In this resolution we explicitly introduce the idea that the functions $\psi^*(x)$ and $\psi(x)$ can be varied independently. When these expansions are plugged into the variational version of Schrödinger's equation we find

$$\delta \left\{ \frac{\hbar^2}{2m} \phi_i (\nabla f_i \nabla f_k) \psi_k + \phi_i V_j (f_i f_j f_k) \psi_k - \phi_i E (f_i f_k) \psi_k \right\} = 0 \quad (3)$$

(summation convention used throughout). In these expressions, the parentheses indicate integration over all space: for example $(f_i f_j f_k) = \int f_i(x) f_j(x) f_k(x) d^3x$. The variational equation is satisfied if it holds for any variation in the coefficients ϕ_i , for example $\phi_i = \delta_{il}$. In this case the variational equation becomes a “simple” matrix equation:

$$\mathcal{M}_{ik} \psi_k = 0 \quad \text{where} \quad \mathcal{M}_{ik} = \mathcal{K}_{ik} + \mathcal{V}_{ik} - E \mathcal{S}_{ik} \quad \text{and} \quad \begin{aligned} \mathcal{K}_{ik} &= (\nabla f_i \nabla f_j) \\ \mathcal{V}_{ik} &= V_j(f_i f_j f_k) \\ \mathcal{S}_{ik} &= (f_i f_k) \end{aligned} \quad (4)$$

Construction of the Kinetic Energy, Potential Energy, and Overlap Matrices $(\mathcal{K}, \mathcal{V}, \mathcal{S})$ becomes almost straightforward with appropriate choices of the basis functions $f_i(x)$.

3 Tessellation

It is useful to divide the configuration space under consideration into small units. The most convenient units are *simplices*. In D dimensions these small building blocks are line segments ($D = 1$), triangles ($D = 2$), and tetrahedra ($D = 3$). A D -dimensional simplex is specified by its $D + 1$ vertices. For example, a line segment in R^1 is defined by its two end points a and b . Triangles in a plane are defined by their three vertices $(a_1, a_2), (b_1, b_2), (c_1, c_2)$. And tetrahedron in R^3 are defined by their four vertices $(a_1, a_2, a_3), (b_1, b_2, b_3), (c_1, c_2, c_3), (d_1, d_2, d_3)$. It is useful to identify simplices with special determinants:

$$\Delta(a, b) = \begin{vmatrix} a & 1 \\ b & 1 \end{vmatrix} \quad \Delta(\mathbf{a}, \mathbf{b}, \mathbf{c}) = \begin{vmatrix} a_1 & a_2 & 1 \\ b_1 & b_2 & 1 \\ c_1 & c_2 & 1 \end{vmatrix} \quad \Delta(\mathbf{a}, \mathbf{b}, \mathbf{c}, \mathbf{d}) = \begin{vmatrix} a_1 & a_2 & a_3 & 1 \\ b_1 & b_2 & b_3 & 1 \\ c_1 & c_2 & c_3 & 1 \\ d_1 & d_2 & d_3 & 1 \end{vmatrix} \quad (5)$$

The volume of a D -dimensional simplex is the determinant of the corresponding $(D + 1) \times (D + 1)$ matrix, divided by $D!$. For example, the volume of the tetrahedron with vertices at $\mathbf{a}, \mathbf{b}, \mathbf{c}, \mathbf{d}$ is $\frac{1}{3!} \Delta(\mathbf{a}, \mathbf{b}, \mathbf{c}, \mathbf{d})$.

4 Basis Functions

A simple and convenient set of basis functions consists of the set of piecewise linear functions that assume the value +1 on one vertex and drop to zero linearly at all the other vertices of simplices sharing this vertex. Such functions are conveniently represented as ratios of determinants. For example, in 2 dimensions the function $f_{\mathbf{b},(\mathbf{a},\mathbf{c})}(x, y)$ on the simplex with vertices \mathbf{a}, \mathbf{b} and \mathbf{c} is obtained from $\Delta(\mathbf{a}, \mathbf{b}, \mathbf{c})$ by replacing row \mathbf{b} by $\mathbf{x} = (x, y)$ and dividing through by $\Delta(\mathbf{a}, \mathbf{b}, \mathbf{c})$:

$$f_{\mathbf{b},(\mathbf{a},\mathbf{c})}(x, y) = \Delta(\mathbf{a}, \mathbf{x}, \mathbf{c}) / \Delta(\mathbf{a}, \mathbf{b}, \mathbf{c}) = \begin{vmatrix} a_1 & a_2 & 1 \\ x & y & 1 \\ c_1 & c_2 & 1 \end{vmatrix} \div \begin{vmatrix} a_1 & a_2 & 1 \\ b_1 & b_2 & 1 \\ c_1 & c_2 & 1 \end{vmatrix} \quad (6)$$

The function $f_{\mathbf{b},(\mathbf{a},\mathbf{c})}(x, y)$ is +1 at the vertex \mathbf{b} and falls linearly to zero at vertices \mathbf{a} and \mathbf{c} . It is defined to be zero outside the simplex $\mathbf{a}, \mathbf{b}, \mathbf{c}$.

This function is linear in x and y over the simplex $\mathbf{a}, \mathbf{b}, \mathbf{c}$. Its gradient therefore has x - and y -components components obtained by replacing $(x, y, 1) \rightarrow (1, 0, 0)$ and $(x, y, 1) \rightarrow (0, 1, 0)$, resp:

$$\Delta(\mathbf{a}, \mathbf{b}, \mathbf{c}) \nabla f_{\mathbf{b},(\mathbf{a},\mathbf{c})}(x, y) = \begin{vmatrix} a_1 & a_2 & 1 \\ 1 & 0 & 0 \\ c_1 & c_2 & 1 \end{vmatrix} \mathbf{e}_1 + \begin{vmatrix} a_1 & a_2 & 1 \\ 0 & 1 & 0 \\ c_1 & c_2 & 1 \end{vmatrix} \mathbf{e}_2 \quad (7)$$

This result holds generally, and simplifies computation of the kinetic energy matrix \mathcal{K} .

The basis function at a point is the union (or sum) of basis functions on all simplices sharing that point. Such a union has value +1 at the point and drops off linearly within each simplex as the other vertices are approached. If, for example, five triangles share a common vertex at \mathbf{a} and have $\mathbf{d}_1, \mathbf{d}_2, \mathbf{d}_3, \mathbf{d}_4, \mathbf{d}_5$ as their other defining vertices, then

$$f_{\mathbf{a}}(x, y) = f_{\mathbf{a},(\mathbf{d}_1,\mathbf{d}_2)}(x, y) + f_{\mathbf{a},(\mathbf{d}_2,\mathbf{d}_3)}(x, y) + f_{\mathbf{a},(\mathbf{d}_3,\mathbf{d}_4)}(x, y) + f_{\mathbf{a},(\mathbf{d}_4,\mathbf{d}_5)}(x, y) + f_{\mathbf{a},(\mathbf{d}_5,\mathbf{d}_1)}(x, y) \quad (8)$$

and the function $f_{\mathbf{a}}\psi_{\mathbf{a}}$ is the function whose value is $\psi_{\mathbf{a}}$ at the vertex \mathbf{a} and which decreases linearly to 0 at the five vertices $\mathbf{d}_1, \mathbf{d}_2, \mathbf{d}_3, \mathbf{d}_4, \mathbf{d}_5$. It is not differentiable at any vertex or on edges joining any two vertices. This does not create a problem for treatment of the Schrödinger equation.

The value of the wavefunction $\psi(x)$ (and potential $V(x)$) is approximated by a discrete set of numbers $\psi_{\mathbf{a}}$ through the superposition

$$\psi(x, y) = \sum_{\text{all } \mathbf{a}} \psi_{\mathbf{a}} f_{\mathbf{a}}(x, y) \quad (9)$$

where $f_{\mathbf{a}}(x, y)$ is a function of the type described by Eq.(.).

5 Important Integrals

Functions $f_{\mathbf{a}}$ depend on the nature of the tessellation, so that integrals of these functions with others of this type change from problem to problem, and even for the same problem with different tessellations. Integrals of functions defined only on a single simplex such as $f_{\mathbf{a},(\mathbf{b},\mathbf{c})}(x, y)$ do not suffer this problem. They are proportional only to the volume of the simplex, or to the determinant of the associated matrix.

For this reason it is useful to compile a table of values of integrals involving such functions. These integrals vanish unless indices i and j “belong” to the same simplex. If they do, (f_i, f_j) has one value if f_i and f_j assume value +1 at the same vertex (it doesn’t matter which) and a different value if they assume values +1 at different vertices (again, it doesn’t matter). Similar statements hold for integrals of three functions f_i . The results are summarized in Table 1. The various possible cases are summarized using the notation of Young partitions: (2,0) means that both functions on the same simplex have values +1 at the same vertex and (1,1) means that they have values +1 at different vertices. In the case of integrals over three functions the possibilities are: (3,0) — all three functions are identical; (2,1) — two are identical and one is different; (1,1,1) — all three functions reach +1 at different vertices (not possible in 1 dimension).

Gradients are inversely proportional to the determinant and independent of coordinates. As a result, they are given by inner products of determinants of the form shown in Eq.(??), divided by $\Delta(*)^2$, and multiplied by the volume, $\Delta/D!$. As a result, $(\nabla f_i \nabla f_j) = D! \Delta(*) \times$ dot product of two determinants. For example

Table 1: Integrals involving two and three functions over a single simplex are proportional to the volume of the simplex, and therefore the determinant associated with the simplex. The integrals depend on whether the functions are +1 at the same vertex or different vertices. All integrals are normalized by the corresponding determinant.

	$D = 1$	$D = 2$	$D = 3$
	$(f_i f_j)/\Delta(a, b)$	$(f_i f_j)/\Delta(\mathbf{a}, \mathbf{b}, \mathbf{c})$	$(f_i f_j)/\Delta(\mathbf{a}, \mathbf{b}, \mathbf{c}, \mathbf{d})$
(2, 0)	1/3	1/6	1/10
(1, 1)	1/6	1/12	1/20
	$(f_i f_j f_k)/\Delta(a, b)$	$(f_i f_j f_k)/\Delta(\mathbf{a}, \mathbf{b}, \mathbf{c})$	$(f_i f_j f_k)/\Delta(\mathbf{a}, \mathbf{b}, \mathbf{c}, \mathbf{d})$
(3, 0)	1/4	1/10	1/20
(2, 1)	1/12	1/30	1/60
(1, 1, 1)	---	1/60	1/120

$$\begin{aligned}
2!\Delta(\mathbf{a}, \mathbf{b}, \mathbf{c})(\nabla f_{\mathbf{a},(\mathbf{b},\mathbf{c})}\nabla f_{\mathbf{b},(\mathbf{a},\mathbf{c})}) &= \begin{vmatrix} 1 & 0 & 0 \\ b_1 & b_2 & 1 \\ c_1 & c_2 & 1 \end{vmatrix} \begin{vmatrix} a_1 & a_2 & 1 \\ 1 & 0 & 0 \\ c_1 & c_2 & 1 \end{vmatrix} + \begin{vmatrix} 0 & 1 & 0 \\ b_1 & b_2 & 1 \\ c_1 & c_2 & 1 \end{vmatrix} \begin{vmatrix} a_1 & a_2 & 1 \\ 0 & 1 & 0 \\ c_1 & c_2 & 1 \end{vmatrix} \\
&= (b_2 - c_2) (c_2 - a_2) + (c_1 - b_1) (a_1 - c_1)
\end{aligned} \tag{10}$$

In one dimension $(b-a)(\nabla f_{a,(b)}\nabla f_{a,(b)}) = (b-a)(\nabla f_{b,(a)}\nabla f_{b,(a)}) = +1$ and $(b-a)(\nabla f_{a,(b)}\nabla f_{b,(a)}) = -1$.

6 One-Dimension

We illustrate this method first with a simple one-dimensional problem. The potential is local and assumed to be $V(x)$. The interval is divided into simplices. In this case the simplices are subintervals. The endpoints of these intervals are indexed by integers i ($i \leftrightarrow x_i$) and the subinterval between i and $i+1$ has length $\Delta_{i,i+1} = x_{i+1} - x_i$. The subintervals do not necessarily have equal lengths. The potential $V(x)$ is represented by the values of the discrete set V_i by means of

$$V(x) = \sum_i V_i f_i(x) \quad f_i(x) = f_{i,(i-1)}(x) + f_{i,(i+1)}(x) \tag{11}$$

The function $f_i(x)$ is +1 at x_i and drops off linearly to zero at the adjacent vertex $i-1$ (courtesy of $f_{i,(i-1)}(x)$) which is 0 on $(i, i+1)$ and also drops off linearly from +1 at i to 0 at $i+1$ courtesy of $f_{i,(i+1)}(x)$.

The i^{th} row of the overlap matrix is

$$\mathcal{S}_{ij} \rightarrow \dots, \frac{\Delta_{i-1,i}}{6}, \frac{\Delta_{i-1,i}}{3}, \frac{\Delta_{i,i+1}}{3}, \frac{\Delta_{i,i+1}}{6}, \dots \tag{12}$$

The i^{th} row of the potential energy matrix is

$$\mathcal{V}_{ij} \rightarrow \dots, \frac{V_{i-1} + V_i}{12} \Delta_{i-1,i}, \left(\frac{V_{i-1}}{12} + \frac{V_i}{4} \right) \Delta_{i-1,i} + \left(\frac{V_i}{4} + \frac{V_{i+1}}{12} \right) \Delta_{i,i+1}, \frac{V_i + V_{i+1}}{12} \Delta_{i,i+1}, \dots \quad (13)$$

Finally, the i^{th} row of the kinetic energy matrix is

$$\mathcal{K}_{ij} \rightarrow \dots, -\frac{1}{\Delta_{i-1,i}}, \frac{1}{\Delta_{i-1,i}} + \frac{1}{\Delta_{i,i+1}}, -\frac{1}{\Delta_{i,i+1}}, \dots \quad (14)$$

Each of the three matrices $\mathcal{K}, \mathcal{V}, \mathcal{S}$ is symmetric (always). In this simple one-dimensional case each matrix is also tridiagonal.

7 Boundary Conditions

The first problem treated in most Quantum Mechanics texts is a particle confined to a one-dimensional box. For such problems, the potential is assumed to be finite (usually 0) from $x = 0$ to $x = a$ and infinitely high outside this region. The boundary conditions are $\psi(x = 0) = 0$ and $\psi(x = a) = 0$. This translates, in Matrix Mechanics language, to the vanishing of the coefficients of ψ at the boundary vertices. If the simplex coordinates are $0 \leq i \leq N + 1$ so that $x_i = i \times a / (N + 1)$, then the boundary conditions force $\psi_0 = 0$ and $\psi_{N+1} = 0$. The matrix to be diagonalized is the $N \times N$ matrix $\mathcal{K} + \mathcal{V} - SE$ and its eigenvectors $(\psi_1, \psi_2, \dots, \psi_N)^t$ provide the approximations to the various eigenfunctions $\psi(x)$.

Many pertinent problems have no discontinuity in the potential. Instead, the potential is finite (perhaps very large) for all interesting values of x . Two useful examples are the harmonic potential $V(x) = \frac{k}{2}x^2$ and the Ginzburg-Landau potential $V(x) = -\frac{\lambda}{2}x^2 + \frac{1}{4}x^4$. In such cases a finite length along the x axis is chosen (for example, $-L \leq x \leq +L$) and divided into segments. The boundary values ψ_0 and ψ_N , where $i = 0$ indexes $x = -L$ and $i = N$ indexes $x = +L$, are not forced to be zero and are retained in the computation. An $(N + 1) \times (N + 1)$ matrix is diagonalized. Eigenfunctions for which the boundary components ψ_0 and ψ_N are both approximately zero are candidates for good approximations to the eigenvalues $\psi(x)$ of the original Schrödinger equation. Those eigenvectors of the matrix diagonalization where either of the boundary values for ψ is nonzero must be rejected as candidates for proper wavefunctions. There must always be eigenfunctions whose boundary values are nonzero, since eigenfunctions are forcibly orthogonal. As a result, the key to successful use of finite-dimensional matrix diagonalizations as an approximation to Wave Mechanics is determining where to draw the line between good and bad approximations to spatial eigenfunctions $\psi(x)$.

8 Two Dimensions

As our first two-dimensional problem we consider a particle of mass m confined to an infinitely deep triangular shaped potential well. The triangle has vertices at the origin $(x, y) = (0, 0) = \mathbf{a}$, along the x -axis at $(b, 0) = \mathbf{b}$, and a distance h above the x -axis at $(a, h) = \mathbf{c}$:

$$\mathbf{a} = (0, 0) \quad \mathbf{b} = (b, 0) \quad \mathbf{c} = (a, h)$$

The determinant, function $f_{\mathbf{a},(\mathbf{b},\mathbf{c})}(x, y)$, and partial derivative $\partial f_{\mathbf{a},(\mathbf{b},\mathbf{c})}(x, y) / \partial y$ are

$$\Delta(\mathbf{a}, \mathbf{b}, \mathbf{c}) = \begin{vmatrix} 0 & 0 & 1 \\ b & 0 & 1 \\ a & h & 1 \end{vmatrix} \quad f_{\mathbf{a},(\mathbf{b},\mathbf{c})}(x, y) = \frac{\begin{vmatrix} x & y & 1 \\ b & 0 & 1 \\ a & h & 1 \end{vmatrix}}{\Delta(\mathbf{a}, \mathbf{b}, \mathbf{c})} \quad \frac{\partial f_{\mathbf{a},(\mathbf{b},\mathbf{c})}(x, y)}{\partial y} = \frac{\begin{vmatrix} 0 & 1 & 0 \\ b & 0 & 1 \\ a & h & 1 \end{vmatrix}}{\Delta(\mathbf{a}, \mathbf{b}, \mathbf{c})} \quad (15)$$

$$bh \qquad \frac{(a-b)y + h(b-x)}{bh} \qquad \frac{a-b}{bh}$$

The triangle will be partitioned into smaller simplices as follows. Each of the three edges is divided into N subintervals of the same length along the respective edges. $(N-1)$ lines are drawn parallel to one side through pairs of points along the other two edges. This is done for each of the three edges. The decomposition is shown in Fig. 1 for $N=5$.

This decomposition results in N^2 smaller triangles and a total of $(N+1)(N+2)/2$ vertices. The smaller triangles are all congruent to each other, and similar to the original triangle. As a result, the integrals for the smaller triangles are all proportional to the integrals for the larger triangle.

For the large triangle these integrals are multiplied by $\Delta(\mathbf{a}, \mathbf{b}, \mathbf{c}) = bh$ (Table 1):

$$\begin{aligned} \Delta(\mathbf{a}, \mathbf{b}, \mathbf{c}) &= bh & (f_{\mathbf{a}}f_{\mathbf{a}}) &= bh/6 & (f_{\mathbf{a}}f_{\mathbf{b}}) &= bh/12 \\ (f_{\mathbf{a}}f_{\mathbf{a}}f_{\mathbf{a}}) &= bh/10 & (f_{\mathbf{a}}f_{\mathbf{a}}f_{\mathbf{b}}) &= bh/30 & (f_{\mathbf{a}}f_{\mathbf{b}}f_{\mathbf{c}}) &= bh/60 \end{aligned} \quad (16)$$

For the large triangle the gradient integrals are divided by $2\Delta(\mathbf{a}, \mathbf{b}, \mathbf{c}) = 2bh$ (Eq.(10)):

$$(\nabla f_i \nabla f_j) \rightarrow \begin{array}{c|ccc} & \nabla f_{\mathbf{a},(\mathbf{b},\mathbf{c})} & \nabla f_{\mathbf{b},(\mathbf{a},\mathbf{c})} & \nabla f_{\mathbf{c},(\mathbf{a},\mathbf{b})} \\ \hline \nabla f_{\mathbf{a},(\mathbf{b},\mathbf{c})} & h^2 + (b-a)^2 & -h^2 + a(b-a) & -b(b-a) \\ \nabla f_{\mathbf{b},(\mathbf{a},\mathbf{c})} & -h^2 + a(b-a) & h^2 + a^2 & -ab \\ \nabla f_{\mathbf{c},(\mathbf{a},\mathbf{b})} & -b(b-a) & -ab & b^2 \end{array} \quad (17)$$

Since $\Delta(\mathbf{a}, \mathbf{b}, \mathbf{c})$ scales like $1/N^2$, the integrals of the functions over the smaller triangles scale like $1/N^2$ and the gradient integrals scale like N^2 .

In going beyond one dimension we lose the linear progression among the indices describing position in the matrices and the D coordinates describing the positions of the vertices. For the regular tessellation shown in Fig. 1 this problem is mitigated with the following strategy. Each coordinate in the plane R^2 is represented by *three* integers i, j, k , with $0 \leq i, j, k \leq N$ and $i + j + k = N$. This indexing is shown in Fig. 1. There is a linear relation between the coordinates (x, y) of a vertex in the tessellated triangle and the triple (i, j, k) :

$$\begin{bmatrix} x \\ y \\ 1 \end{bmatrix} = \begin{bmatrix} D_{1,1} & D_{1,2} & D_{1,3} \\ D_{2,1} & D_{2,2} & D_{2,3} \\ 1/N & 1/N & 1/N \end{bmatrix} \begin{bmatrix} i \\ j \\ k \end{bmatrix} \quad (18)$$

By identifying the vertices $\mathbf{a}, \mathbf{b}, \mathbf{c}$ with triples $(N, 0, 0)$, $(0, N, 0)$, and $(0, 0, N)$, resp., it is a simple matter to determine the matrix elements D_{ij} :

$$\begin{bmatrix} a_1 & b_1 & c_1 \\ a_2 & b_2 & c_2 \\ 1 & 1 & 1 \end{bmatrix} = \begin{bmatrix} D_{1,1} & D_{1,2} & D_{1,3} \\ D_{2,1} & D_{2,2} & D_{2,3} \\ 1/N & 1/N & 1/N \end{bmatrix} \begin{bmatrix} N & 0 & 0 \\ 0 & N & 0 \\ 0 & 0 & N \end{bmatrix} \quad (19)$$

To check whether two vertices belong to the same simplex the differences of their integer coordinates is computed: $(\Delta i, \Delta j, \Delta k)$. If $|\Delta i| + |\Delta j| + |\Delta k|$ is zero, the vertices are the same. If this sum is 2, the vertices belong to the same simplex (two, in fact). Otherwise, they are disjoint and all

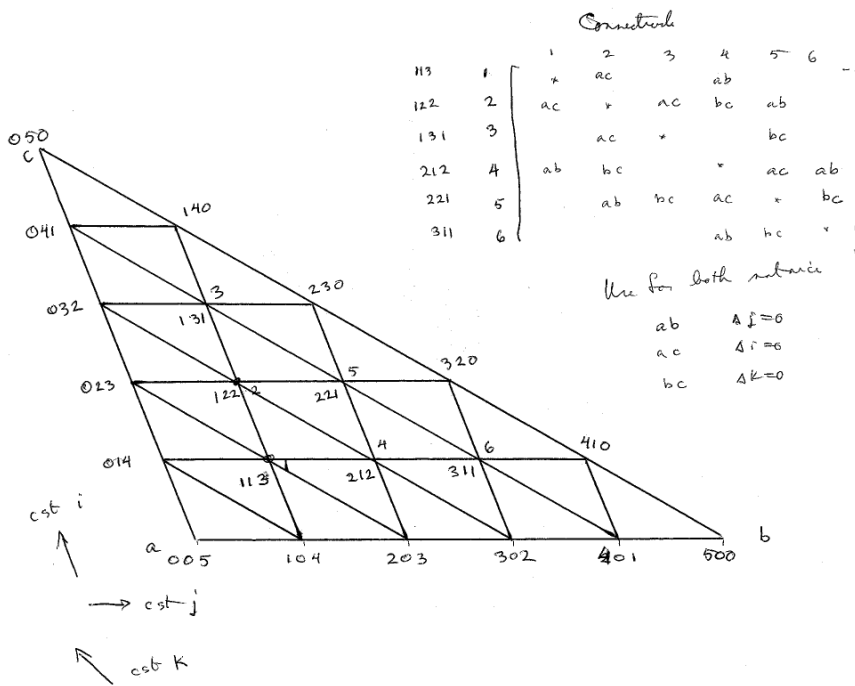


Figure 1: Triangle tessellation.

matrix elements for this pair of vertices are zero. For example, $(2, 0, 3)$ and $(1, 1, 3)$ belong to two simplices while $(2, 0, 3)$ and $(4, 0, 1)$ do not.

When two distinct vertices belong to the same simplex, the edge connecting these vertices is parallel to one of the edges of the initial triangle according to

$$\Delta i = 0 \leftrightarrow \mathbf{ac} \quad \Delta j = 0 \leftrightarrow \mathbf{ab} \quad \Delta k = 0 \leftrightarrow \mathbf{bc} \quad (20)$$

The boundary conditions for this problem are that the wavefunction vanishes at all edges. As a result we set all $\psi_{\mathbf{a}} = 0$ if \mathbf{a} is a boundary vertex in the tessellated triangle. There are $3N$ boundary vertices: \mathbf{v} is a boundary vertex if one of the three integers (i, j, k) in its ternary representation is zero. The result is a set of vertices with ternary representation (i, j, k) with $1 \leq i, j, k \leq N$ and $i + j + k = N$. The total number of vertices is reduced to $(N - 1)(N - 2)/2$. For $N = 5$ this means that a 6×6 matrix must be diagonalized.

In preparation for creating the matrices $\mathcal{S}, \mathcal{K}, \mathcal{V}$ it is useful first to construct a matrix \mathcal{T} (topological matrix or connecting matrix) that identifies just how the coordinates in the tessellation are connected. For the triangle shown in Fig. 1 this matrix is

$$\mathcal{T} = \begin{bmatrix} * & \mathbf{ac} & 0 & \mathbf{ab} & 0 & 0 \\ \mathbf{ac} & * & \mathbf{ac} & \mathbf{bc} & \mathbf{ab} & 0 \\ 0 & \mathbf{ac} & * & 0 & \mathbf{bc} & 0 \\ \mathbf{ab} & \mathbf{bc} & 0 & * & \mathbf{ac} & \mathbf{ab} \\ 0 & \mathbf{ab} & \mathbf{bc} & \mathbf{ac} & * & \mathbf{bc} \\ 0 & 0 & 0 & \mathbf{ab} & \mathbf{bc} & * \end{bmatrix} \leftrightarrow \begin{bmatrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \end{bmatrix} \leftrightarrow \begin{bmatrix} (1, 1, 3) \\ (1, 2, 2) \\ (1, 3, 1) \\ (2, 1, 2) \\ (2, 2, 1) \\ (3, 1, 1) \end{bmatrix} \quad (21)$$

To the right of this matrix are the indices that label the interior vertices of the tessellation. They are given in numerical order in which they index matrices input to and output from a computer, and in triples (i, j, k) satisfying the conditions described above. The relation between the computer indices $n = n(i, j, k)$ and the triples (i, j, k) is

$$(i, j, k) \rightarrow n = \frac{1}{2}(N - 2)(N - 1) - \frac{1}{2}(N - 1 - i)(N - i) + j \quad (22)$$

Going backward from $n(i, j, k)$ to the triple (i, j, k) , subtract $(N - 2)$ from n , then $(N - 3)$, then $(N - 4)$, etc. At each step, check that the remainder is greater than zero. When this test fails, add back the last integer that was subtracted. Then i is the total number of subtractions, j is the integer obtained after the last addition, and $k = N - i - j$.

The nondiagonal entries in \mathcal{T} indicate which edge connects two vertices. For example, \mathbf{ac} indicates that two vertices (e.g., 1 and 2 or $(1, 1, 3)$ and $(1, 2, 2)$) are connected to an edge in a smaller triangle that is similar to the edge \mathbf{ac} of the original triangle. An entry 0 indicates that the two vertices are not contained in any simplex. The larger N , the smaller the ratio of nonzero matrix elements to zero matrix elements - the matrix \mathcal{T} is *sparse*.

At this point a sanity check is useful. This matrix must satisfy a number of symmetries, some transparent and others not so obvious. For example, the number of letters \mathbf{a} in this distribution is $2N$, and similarly for \mathbf{b} and \mathbf{c} . The number of nonzero offdiagonal matrix elements is $3 \times N$.

The nature of the tessellation, which produces a whole bunch of smaller triangles, all congruent to each other and similar by a simple scale factor $(1/N)$ to the original, allows us to “mass-produce” the matrix elements for the overlap matrix \mathcal{S} and the kinetic energy matrix \mathcal{K} . These are constructed by computing the integrals $(f_i f_j)$ and $(\nabla f_i \nabla f_j)$ in the original large triangle, scaling appropriately, and substituting into \mathcal{T} . We reserve introducing the scaling factors until the last step. The substitutions provided in Table 2 are appropriate to convert \mathcal{T} into matrices proportional to \mathcal{S} and \mathcal{K} :

Table 2: Substitutions useful for converting the connectivity matrix \mathcal{T} to matrices \mathcal{S} and \mathcal{K} . Here A is the area of the large triangle: $\frac{1}{2}bh$.

\mathcal{S}		\mathcal{K}			
*	ab, ac, bc	*	ab	ac	bc
$\frac{6}{6}A$	$\frac{2}{12}A$	$2(2h^2 + a^2 + b^2 + (a - b)^2)$	$2(-h^2 + a(b - a))$	$2(-ab)$	$2(-b(b - a))$

We illustrate how this works for the triangle with one vertex at the origin, another along the x -axis at $(2,0)$, and the third in the x - y plane at $(-\frac{1}{2}, 1)$. This triangle has area 1. The 25 smaller triangles have area $1/5^2$. The (unscaled) matrices \mathcal{S} and \mathcal{K} are

$$\mathcal{S}(\text{unscaled}) = \begin{bmatrix} 1 & 1/6 & 0 & 1/6 & 0 & 0 \\ 1/6 & 1 & 1/6 & 1/6 & 1/6 & 0 \\ 0 & 1/6 & 1 & 0 & 1/6 & 0 \\ 1/6 & 1/6 & 0 & 1 & 1/6 & 1/6 \\ 0 & 1/6 & 1/6 & 1/6 & 1 & 1/6 \\ 0 & 0 & 0 & 1/6 & 1/6 & 1 \end{bmatrix} \quad (23)$$

$$\mathcal{K}(\text{unscaled}) = \begin{bmatrix} 25 & 2 & 0 & -9/2 & 0 & 0 \\ 2 & 25 & 2 & -10 & -9/2 & 0 \\ 0 & 2 & 25 & 0 & -10 & 0 \\ -9/2 & -10 & 0 & 25 & 2 & -9/2 \\ 0 & -9/2 & -10 & 2 & 25 & -10 \\ 0 & 0 & 0 & -9/2 & -10 & 25 \end{bmatrix} \quad (24)$$

The eigenvalue equation is obtained by combining these two matrices with the appropriate scaling factors:

$$\left(\frac{5^2}{2} \mathcal{K}(\text{unscaled}) - \frac{2}{5^2} \mathcal{S}(\text{unscaled}) E \right) \psi_i = 0 \quad (25)$$

The scaling factor is $N^{\pm 2}$: $+2$ for the matrix \mathcal{K} and -2 for the matrix \mathcal{S} . The factors 5 ($5^{\pm 2}$) come from the N^2 scaling and the factors 2 are from $\Delta(\mathbf{a}, \mathbf{b}, \mathbf{c})$, where the area of the large triangle is $\frac{1}{2}bh = 1$.

9 Solving the Eigenvalue Equation

10 Improving the Results