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From Wave Mechanics to Matrix Mechanics: The Finite Element Method

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1 The Origin of Wave Mechanics

Schrödinger originally formulated Wave Mechanics as a variational problem:

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

There are only a few analytic solutions available for this partial differential equation. Schrödinger found all of the most useful ones in his first paper on Quantum Mechanics: the Coulomb potential and the harmonic oscillator potential. He published the solution to the nonrelativistic Coulomb problem in his first Wave Mechanics paper but solved the relativistic problem six months earlier. He also solved the harmonic oscillator problem in his first paper and introduced what are now called coherent states in another paper six months afterward.

With the advent of powerful computers and even more powerful linear algebra algorithms, partial differential equations are usually solved by first transforming them into matrix equations and then solving the matrix equations. Solutions almost always involve either matrix inversion or matrix diagonalization.

The Schrödinger equation is usually not given in the original variational form. It is usually expressed as a second order partial differential equation. The relation between the two is obtained as follows. The kinetic energy term is integrated by parts:

$$\int \frac{\nabla\psi^* \cdot \nabla\psi}{2m(x)} dV = \int \nabla\cdot\left(\frac{\psi^* \nabla\psi}{2m(x)} \right) dV - \int \psi^* \nabla\cdot \left(\frac{\nabla\psi}{2m(x)} \right) dV = \int_{\partial V} \left(\frac{\psi^* \nabla\psi}{2m(x)} \right) \cdot d\mathbf{S} - \int \psi^* \nabla\cdot \left(\frac{\nabla\psi}{2m(x)} \right) dV \tag{2}$$

When the surface integral vanishes, the kinetic energy term in the variational expression can be replaced by the negative of the Laplacian. The variational expression is now

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

The functions $\psi(x)$ and $\psi^*(x)$ can be varied independently. Varying $\psi^*(x)$ leads to "the" Schrödinger equation:

$$-\hbar^2 \nabla\cdot \left(\frac{\nabla\psi(x)}{2m(x)} \right) + V(x)\psi - E\psi = 0 \tag{4}$$

When $m(x)$ is a constant this equation assumes its universally recognized form. In many cases the effective mass $m(x)$ is not constant: for example, in solids where the effective mass is a surrogate for

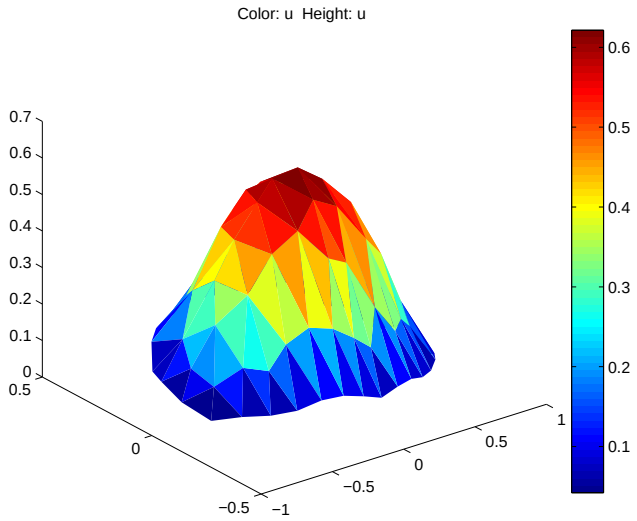

Figure 1: The ground state wavefunction for a particle trapped in an infinitely deep two-dimensional potential well has been evaluated at a small number of points and a 3D plot constructed from the triples of values (x_i, y_i, ψ_i). The wavefunction is linearly interpolated between triples of nearby points. This faceted representation provides an "accurate" understanding of the wavefunction.

many electron effects. In such cases it is important to recognize that continuity conditions across boundaries should be imposed on the wavefunction $\psi(x)$ and on the *velocity* $\nabla\psi(x)/m(x)$, *not* on the momentum $\nabla\psi(x)$.

Today, if we wanted to visualize a wavefunction, we would try to display it on a computer screen. To do this, we would have to determine its value at a discrete set of points $(x, y)_i$ in the plane and then construct a "3D" plot (x_i, y_i, ψ_i), where $\psi_i = \psi(x_i, y_i)$. Many plotting routines routinely interpolate values the the function being plotted between the points at which the function is evaluated. Such a visualization is shown in Fig. 1.

The purpose of Fig. 1 is to emphasize that the eigenfunction is well-represented if its value is known at a lot of nearby points.

The idea underlying the finite element method (in 2D) is to replace the problem of determining the wavefunction $\psi(x, y)$ at all (x, y) (basically by solving a PDE) by the problem of determining only a sample of values ψ_i at a discrete set of points $(x, y)_i$ (basically by solving a matrix eigenvalue equation).

2 Tesselation

The first step in applying the finite element method is to determine the points at which the wavefunction is to be evaluated. To this end the region of space (1D, 2D, 3D, ...) of interest is determined. A boundary is placed on or around this region. Then a set of points is distributed throughout this bounded region, including on the boundary itself. There is a Goldilocks problem here. If too few points are used we will construct a poor representation of the wavefunction. If too many points

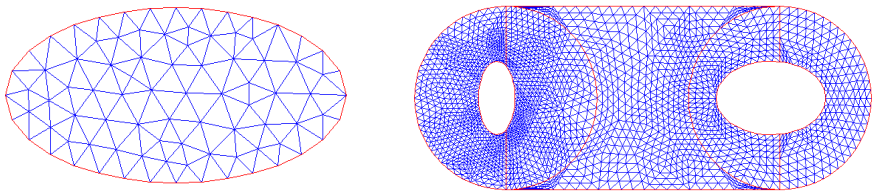

Figure 2: (a) Tesselation of an elliptical region of the plane. The bound ground state shown in Fig. 1 was computed on the basis of this tesselation. (b) This tesselation of a non simply connected arena-shaped area in the plane requires many more vertices than that for the ellipse.

are introduced the matrices we have to deal with will be corresponding large and take too long to diagonalize. With just the "right" number of points, magic happens.

It is typical, and useful, to distribute a higher density of points (called vertices) where it is expected, on inutitive grounds, that the wavefunction will vary more rapidly, and fewer points where lower gradients are anticipated. Once the points have been distributed, nearby points are connected by edges, the edges bound faces, and (in 3D) the faces bound volumes. Such a structure forms a *tesselation* of the domain of interest. Tesselations are not straightforward to construct. We will use tesselations with the property that only *simplices* occur. In 2D these are triangles; in 3D these are tetrahedra; ... .

We illustrate the idea of tesselation in Fig. 2. On the left we show a tesselation of an elliptical region of the plane. This tesselation has very few vertices, and in fact is the tesselation leading to the representation of the ground state wavefunction shown in Fig. 1. On the right in Fig. 2 is an arena shaped area with two interior elliptical forbidden zones. The problem is to compute the ground state of a particle confined to this "box". This is not a problem to be attempted with analytic methods. The tesselation of the allowed area of this bounded region has many more points than the tesselation on its left.

The basic idea of the finite element method is to:

1. Introduce an unknown value of the wavefunction ψ_i at each vertex of the tesselation;
2. Express the value of the action integral in terms of the unknown values ψ_i;
3. Look for the stationary values of the quadratic form that results;
4. Construct the eigenvectors for the matrix expression of the variational problem;
5. Extract the Physics from this Mathematics.

For many purposes the unknown amplitudes ψ_i at each vertex can be assumed to be real. This is true whenever only bound states are of interest. When scattering problems are being treated, or magnetic fields are present, then it is necessary to allow the amplitudes to be complex.

3 Finite Elements

There are several levels of sophistication in which to proceed. We treat the following cases:

Section 3: 2 dimensions, linear basis functions.

Section 4: 3 dimensions, linear basis functions.

Section 5: 2 dimensions, cubic basis functions.

Section 6: 3 dimensions, cubic basis functions.

We first describe a simple case. A potential acts on a particle of mass m in a localized region in 2 D. A region in two dimensions containing the potential is tesselated by choosing a sufficient number of vertices. The vertices are uniquely identified — usually through an integer i that ranges from 1 to N_V. The region is divided into adjacent areas; each area is called an element. The elements are also uniquely identified — usually through an integer α that ranges from 1 to N_E. The three (or more) vertices that define the edges of each element are associated with that element through a list. Another list contains information about the coordinates of each vertex. The behavior of a wavefunction in each element is represented by a linear combination of basis functions that are nonzero only in that element.

If the ultimate objective is to determine the wavefunction, and it is required to have the wavefunction be continuous but there is no concern about having the derivatives across elements be continuous, we are in one domain of simplicity. We describe what happens in this domain and let the complications pile on later.

Within an element with 3 vertices we choose 3 basis functions. Each has value +1 at one of the three vertices and vanishes at the other two. These three functions are defined *only* within that single element. To put it another way, they are defined to be zero outside that specific element.

It is useful in principle to take the three basis functions to be linear combinations of the constant 1 and the coordinates x and y (that is not what we do). If we do this the wave function can be written

$$\psi(x) = \sum_{\alpha=1}^{N_E} \psi_\alpha(x) \tag{5}$$

Here $\psi_\alpha(x)$ is zero outside the element α and nonzero only inside this element. In fact, it linearly interpolates between the (unknown) values of the wavefunction at the three coordinates.

The terms in the variational expression Eq.(1) simplify. For example

$$\int \psi^*(x) E \psi(x) dx = \int \left(\sum_{\alpha=1}^{N_E} \psi_\alpha(x) \right) E \left(\sum_{\beta=1}^{N_E} \psi_\beta(x) \right) dx = E \sum_{\alpha=1}^{N_E} \int \psi_\alpha^*(x) \psi_\alpha(x)\ dx \tag{6}$$

The collapse of the double sum to a single sum in the last equation comes about because $\psi_\alpha(x)$ is zero where $\psi_\beta(x)$ is nonzero, unless $\alpha = \beta$. This is true also for derivatives of either or both of these functions.

The wave function $\psi_\alpha(x)$ will be "cooked up" to interpolate linearly between the values that $\psi(x)$ assumes at the three vertices that define the element α. As a result, $\psi_\alpha(x)$ will depend linearly on these three values, and the expectation value in Eq.(10) will be a quadratic form in these unknowns.

The potential energy term is treated similarly:

$$\int \psi^*(x) V(x) \psi(x) dx = \int \left(\sum_{\alpha=1}^{N_E} \psi_\alpha(x) \right) V(x) \left(\sum_{\beta=1}^{N_E} \psi_\beta(x) \right) dx = \sum_{\alpha=1}^{N_E} \int \psi_\alpha^*(x) V(x) \psi_\alpha(x)\ dx \tag{7}$$

The same goes for the kinetic energy term:

$$\frac{\hbar^2}{2m}\int \nabla\psi^*(x)\nabla\psi(x)dx = \frac{\hbar^2}{2m}\int \left(\sum_{\alpha=1}^{N_E}\nabla\psi_\alpha(x)\right)^* \left(\sum_{\beta=1}^{N_E}\nabla\psi_\beta(x)\right) dx = \frac{\hbar^2}{2m}\sum_{\alpha=1}^{N_E}\int \nabla\psi_\alpha^*(x)\nabla\psi_\alpha(x)\,dx \tag{8}$$

All three expressions, Eqs. (10 - 12), are quadratic forms in the unknown values of the wavefunction at the vertices defining the element α.

This is the general outline. The devil is in the details. So we now illustrate the workings of this method by outlining an example.

4 2D: Linear Functions

The equations above show that there are a lot of integrals to do. Ultimately, each integral will be expressed as a quadratic form in the values of ψ at the vertices, multiplied by some function of the coordinates of the vertices. These fucntions are closely related to each other. to simplify life, we proceed as follows. First we define a benchmark simplex. This will be a right triangle in the $\xi - \eta$ plane. The coordinates of the vertices of this right triangle are $(0,0)$, $(1,0)$, and $(0,1)$ (see Fig. 3). We take as three basis functions in this benchmark triangle

$$\begin{array}{rcl} \phi_0 &=& 1-\xi-\eta \\ \phi_1 &=& \xi \\ \phi_2 &=& \eta \end{array} \tag{9}$$

These three functions have the desired properties

	Value at $(0,0)$	Value at $(1,0)$	Value at $(0,1)$
$\phi_0(\xi,\eta)$	1	0	0
$\phi_1(\xi,\eta)$	0	1	0
$\phi_2(\xi,\eta)$	0	0	1

(10)

The integrals in Eqs. (10 - 12) are most simply done by using the chain rule to change variables. The change of variables is a simple linear transformation, so the integrals can be transformed from the "real" (x,y) space to the "benchmark" (ξ,η) space, where they need be worked out only once. Since the transformation is linear, the jacobian of the transformation is a constant that can be removed from all integrals.

4.1 Structure of Approximation

Here goes. Set up 3 matrices. Each is $N_V \times N_V$ in size, with rows and columns labeled by the index (i) used to identify the different vertices.

Choose an element, say $\alpha = 19$. From the list of elements and their vertices, determine the 3 vertices associated with element 19. Let's say they are 3, 5, and 9. Change variables from (x,y) to (ξ,η) as follows:

$$\begin{array}{rcl} (x,y)_3 &\rightarrow& (0,0) \\ (x,y)_9 &\rightarrow& (1,0) \\ (x,y)_5 &\rightarrow& (0,1) \end{array} \qquad \xi = \frac{\begin{vmatrix} x-x_3 & y-y_3 \\ x_5-x_3 & y_5-y_3 \end{vmatrix}}{\begin{vmatrix} x_9-x_3 & y_9-y_3 \\ x_5-x_3 & y_5-y_3 \end{vmatrix}} \qquad \eta = \frac{\begin{vmatrix} x_9-x_3 & y_9-y_3 \\ x-x_3 & y-y_3 \end{vmatrix}}{\begin{vmatrix} x_9-x_3 & y_9-y_3 \\ x_5-x_3 & y_5-y_3 \end{vmatrix}} \tag{11}$$

At this point it is very useful to express the linear transformation between coordinates (x, y) in the physical space and the coordinates (ξ, η) in the benchmark space in terms of the 2×2 matrix $[J]$ whose determinant appears in the denominators above:

$$\begin{pmatrix} x - x_3 & y - y_3 \end{pmatrix} = \begin{pmatrix} \xi & \eta \end{pmatrix} \begin{bmatrix} x_9 - x_3 & y_9 - y_3 \\ x_5 - x_3 & y_5 - y_3 \end{bmatrix} \leftrightarrow \begin{bmatrix} \partial/\partial\xi \\ \partial/\partial\eta \end{bmatrix} = \begin{bmatrix} x_9 - x_3 & y_9 - y_3 \\ x_5 - x_3 & y_5 - y_3 \end{bmatrix} \begin{bmatrix} \partial/\partial x \\ \partial/\partial y \end{bmatrix} \tag{12}$$

The dual relation that exists between transformations of coordinates and derivatives with respect to these coordinates is a consequence of co- and contra-variance.

Next, we approximate $\psi(x, y)$ within element 19 by a linear combination of the benchmark functions within the benchmark triangle:

$$\psi_{19}(x, y) \to \psi_3\phi_0(\xi, \eta) + \psi_9\phi_1(\xi, \eta) + \psi_5\phi_2(\xi, \eta) \tag{13}$$

The three coefficients(ψ_3, ψ_9, ψ_5) are at present unknown, as are all the other values ψ_i of $\psi(x, y)$ at the vertices.

4.2 Matrix of Overlap Integrals

Now we compute $\int |\psi_{19}(x, y)|^2 dx \wedge dy$ over the element 19 by exploiting the linear change of variables:

$$\int \psi_{19}(x, y)^2 dx \wedge dy = \int \left(\psi_3\phi_0(\xi, \eta) + \psi_9\phi_1(\xi, \eta) + \psi_5\phi_2(\xi, \eta)\right)^2 \frac{dx \wedge dy}{d\xi \wedge d\eta}\, d\xi \wedge d\eta \tag{14}$$

Since ξ and η are linear in x and y the jacobian $\frac{dx \wedge dy}{d\xi \wedge d\eta} = |J|$ is constant. This is the ratio of the physical triangle with vertices $3, 9, 5$ to the benchmark right triangle with vertices $0, 1, 2$. The absolute value of this constant may be taken out of the integral. Remaining inside the integral are bilinear products of the three functions $\phi_k(\xi, \eta)$ and bilinear products of the three unknowns ψ_i and their complex conjugates. The functions of (ξ, η) can be integrated once and for all. The matrix of inner products is

$$\int\int \phi_i(\xi, \eta)\phi_j(\xi, \eta)\, d\xi \wedge d\eta = \begin{bmatrix} \frac{1}{12} & \frac{1}{24} & \frac{1}{24} \\ \frac{1}{24} & \frac{1}{12} & \frac{1}{24} \\ \frac{1}{24} & \frac{1}{24} & \frac{1}{12} \end{bmatrix} \tag{15}$$

Putting all these results together, the contribution to the overlap matrix from vertices $(3, 9, 5)$ of element 19 is:

$$\frac{1}{24} \left| \begin{matrix} x_9 - x_3 & y_9 - y_3 \\ x_5 - x_3 & y_5 - y_3 \end{matrix} \right| \times \begin{bmatrix} \psi_3 & \psi_9 & \psi_5 \end{bmatrix}^* \begin{bmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{bmatrix} \begin{bmatrix} \psi_3 \\ \psi_9 \\ \psi_5 \end{bmatrix} \tag{16}$$

It remains to place the nine numbers that occur in this 3×3 matrix onto the right places in the large $N_V \times N_V$ matrix representing $\int\int \psi^*(x, y)\ E\ \psi(x, y)\ dx \wedge dy$.

Remark: For bound states the wave functions can be taken real, so the bilinear form in the amplitudes ψ_i^*, ψ_j can be taken as a quadratic form in the real amplitudes ψ_j. This is true for bound states. For scattering states, and when magnetic fields are present, the amplitudes ψ_i are in general complex and cannot be made real.

4.3 Potential Energy Matrix

A similar procedure is followed to compute the potential energy matrix. The left-hand side of Eq.(18) is altered by the includsion of the potential energy, $V(x,y)$. This change propagates to the right hand side of that equation. Under a change of variables, and under the restriction to the same element 19, $\psi(x,y) \to \psi_{19}(\xi,\eta)$ as before and $V(x,y) \to V(\xi,\eta)$. The specified integrals $\psi_\alpha(\xi,\eta)V(\xi,\eta)\psi_\beta(\xi,\eta)$ can then all be carried out by whatever means are desirable (in principle). However, it is useful not to be too careful with these calculations, as a piecewise linear approximation (to the wavefunction) is already in play. It makes sense, and speeds up the calculations, to make a similar approximation for the potential. If V_3, V_9, V_5 are the values of the potential at the corresponding nodes, we have the following integral to perform

$$\int \left(\psi_3\phi_0(\xi,\eta) + \psi_9\phi_1(\xi,\eta) + \psi_5\phi_2(\xi,\eta)\right)^2 \left(V_3\phi_0(\xi,\eta) + V_9\phi_1(\xi,\eta) + V_5\phi_2(\xi,\eta)\right) \frac{dx\wedge dy}{d\xi\wedge d\eta}\; d\xi\wedge d\eta \tag{17}$$

It is evident that many of the processes indicated by this equation have already been carried out. The major difference is that *tri*linear, rather than *bi*linear products of the benchmark functions occur in this integral:

$$I_{\alpha,\beta,\gamma} = \int\int \phi_\alpha(\xi,\eta)\phi_\beta(\xi,\eta)\phi_\gamma(\xi,\eta)\; d\xi\wedge d\eta \tag{18}$$

These have the expected symmetries. The results can be "labeled" by Young partitions: (3) in the case that all three indices are the same, $(2,1)$ in the case that all only two are the same, and $(1,1,1)$ in the case that all three indices are different. The results are

$$\begin{array}{lcccc} (3) & = & 1/20 & = & 6/120 \\ (2,1) & = & 1/60 & = & 2/120 \\ (1,1,1) & = & 1/120 & = & 1/120 \end{array} \tag{19}$$

The 3×3 potential energy matrix for this element is still a quadratic form in the unknown amplitudes ψ_i. It is constructed following the steps leading from Eq.(18) to Eq.(20). The result is

$$\frac{1}{120}\left|\begin{array}{cc} x_9-x_3 & y_9-y_3 \\ x_5-x_3 & y_5-y_3 \end{array}\right| \times \left[\begin{array}{ccc} \psi_3 & \psi_9 & \psi_5 \end{array}\right] \left[\begin{array}{ccc} 6V_3+2V_9+2V_5 & 2V_3+2V_9+1V_5 & 2V_3+1V_9+2V_5 \\ 2V_3+2V_9+1V_5 & 2V_3+6V_9+2V_5 & 1V_3+2V_9+2V_5 \\ 2V_3+1V_9+2V_5 & 1V_3+2V_9+2V_5 & 2V_3+2V_9+6V_5 \end{array}\right] \left[\begin{array}{c} \psi_3 \\ \psi_9 \\ \psi_5 \end{array}\right] \tag{20}$$

It remains to place the nine numbers that occur in this 3×3 matrix onto the right places in the large $N_V \times N_V$ matrix representing $\int\int \psi^*(x,y)\; V(x,y)\; \psi(x,y)\; dx\wedge dy$.

Remark: If a factor of $\frac{1}{2}$ is associated with the jacobian (the area of the triangle), and $\frac{1}{60}$ with the 3×3 matrix, then the sum of all the matrix elements in this matrix is $\frac{1}{60}(20V_3+20V_9+20V_5)$ represents a sophisticated average of the potential over the element.

4.4 Kinetic Energy Matrix

The kinetic energy matrix is built up from yet another variation of Eq.(18):

$$\frac{\hbar^2}{2m}\int \left(\nabla\psi_{19}(x,y)\right)^2 dx\wedge dy \tag{21}$$

The components of the gradient are computed using the chain rule: that is, the linear relation among partial derivatives given is Eq.(16). We apply the column vector of physical derivatives to the function $\psi(x,y)$ and the column vector of benchmark derivatives $\partial/\partial\xi, \partial/\partial\eta$ to the representation $\psi_3\phi_0(\xi,\eta) + \psi_9\phi_1(\xi,\eta) + \psi_5\phi_2(\xi,\eta)$, obtaining

$$\begin{bmatrix} \partial\psi/\partial x \\ \partial\psi/\partial y \end{bmatrix} = J^{-1} \begin{bmatrix} \psi_9 - \psi_3 \\ \psi_5 - \psi_3 \end{bmatrix} \tag{22}$$

The inner product of the gradient of the wavefunction with itself is

$$(\nabla\psi)\cdot(\nabla\psi) = \begin{bmatrix} \partial\psi/\partial x & \partial\psi/\partial y \end{bmatrix} \begin{bmatrix} \partial\psi/\partial x \\ \partial\psi/\partial y \end{bmatrix} = \begin{bmatrix} \psi_9 - \psi_3 & \psi_5 - \psi_3 \end{bmatrix} (J^{-1})^t J^{-1} \begin{bmatrix} \psi_9 - \psi_3 \\ \psi_5 - \psi_3 \end{bmatrix} \tag{23}$$

If we define matrix elements A, B, C of the real symmetric matrix $(J^{-1})^t J^{-1} = (JJ^t)^{-1}$ as described below, the conversion to a 3×3 matrix of the quadratic form for the three coefficients ψ_3, ψ_9, ψ_5 is quickly determined:

$$\begin{bmatrix} \psi_9 - \psi_3 & \psi_5 - \psi_3 \end{bmatrix} \begin{bmatrix} A & B \\ B & C \end{bmatrix} \begin{bmatrix} \psi_9 - \psi_3 \\ \psi_5 - \psi_3 \end{bmatrix} = \begin{bmatrix} \psi_3 & \psi_9 & \psi_5 \end{bmatrix} \begin{bmatrix} A+2B+C & -A-B & -B-C \\ -A-B & A & B \\ -B-C & B & C \end{bmatrix} \begin{bmatrix} \psi_3 \\ \psi_9 \\ \psi_5 \end{bmatrix} \tag{24}$$

This constant must be integrated over the area of simplex 19 with vertices 3, 9, 5. The volume is $\frac{1}{2!}|J|$. The 9 elements in this 3×3 matrix are constructed by computing the matrix J, inverting the matrix JJ^t, and spreading out the $4 = 2^2$ elements of this symmetric matrix in the proper way to construct the $9 = 3^2$ matrix elements for the kinetic energy contribution on element 19. All matrix elements must be multiplied by the positive area factor $\frac{1}{2!}|J|$.

It remains to place the nine numbers that occur in this 3×3 matrix in Eq.(28) onto the right places in the large $N_V \times N_V$ matrix representing $\frac{\hbar^2}{2m} \int\int (\nabla\psi(x,y))^* (\nabla\psi(x,y))\ dx \wedge dy$.

Remark 1: The procedure for constructing the matrix in Eq.(28) is algorithmic in five simple steps.

1. Construct a jacobian matrix as the difference in the x and y coordinates of the triple of vertices defining a triangular element, as shown in Eq.(16).
2. Construct the transpose of this matrix.
3. Compute the product (JJ^t).
4. Compute the inverse of this 2×2 matrix.
5. Spread the 4 matrix elements of this inverse out into 9 matrix elements, as shown in Eq.(28).

This is a very fast and efficient algorithm.

Remark 2: This result is aesthetically unsatisfying in that it appears to treat the three vertices asymmetrically. The result *is* symmetric in the coordinates, despite the appearance of Eq.(28). To show this it is useful to write down the explicit form the the three independent matrix elements A, B, C in terms of the 2 coordinates of each of the 3 vertices: $A = \mathbf{\Delta x}_{20}\cdot\mathbf{\Delta x}_{20}$, $C = \mathbf{\Delta x}_{01}\cdot\mathbf{\Delta x}_{01}$, $B = -\mathbf{\Delta x}_{10}\cdot\mathbf{\Delta x}_{20}$. Here, to reduce complexity of notation, the three vertices are labeled 1, 2, 3 and $\mathbf{\Delta x}_{21}\cdot\mathbf{\Delta x}_{31} = (x_2 - x_1)(x_3 - x_1) + (y_2 - y_1)(y_3 - y_1)$, etc. When these expressions are placed into the 3×3 matrix in Eq.(28), the form for the 11, $1i$, and $i1$ matrixd elements immediately suggests itself:

$$\begin{bmatrix} +\mathbf{\Delta x}_{23}\cdot\mathbf{\Delta x}_{23} & -\mathbf{\Delta x}_{13}\cdot\mathbf{\Delta x}_{23} & -\mathbf{\Delta x}_{12}\cdot\mathbf{\Delta x}_{32} \\ -\mathbf{\Delta x}_{23}\cdot\mathbf{\Delta x}_{13} & +\mathbf{\Delta x}_{31}\cdot\mathbf{\Delta x}_{31} & -\mathbf{\Delta x}_{21}\cdot\mathbf{\Delta x}_{31} \\ -\mathbf{\Delta x}_{32}\cdot\mathbf{\Delta x}_{12} & -\mathbf{\Delta x}_{31}\cdot\mathbf{\Delta x}_{21} & +\mathbf{\Delta x}_{12}\cdot\mathbf{\Delta x}_{12} \end{bmatrix} \tag{25}$$

This matrix is symmetric in the coordinates of the vertex triple!

Remark 3: The local 3×3 kinetic energy matrix should be multiplied by a constant $(\hbar^2/2m)$ before it is placed in the $N_V \times N_V$ kinetic energy matrix. If the mass m is the same in all elements, this multiplication can be postponed until the entire $N_V \times N_V$ kinetic energy matrix is constructed, and then this multiplication can be carried out. On the other hand, if $m = m(x)$ is not the same throughout the region of interest, then multiplication by $\hbar^2/2m_{\text{element}}$ must be carried out on an element by element basis.

4.5 Magnetic Matrix

An additional contribution is necessary when magnetic fields are present. If spin is not explicitly taken into account, all magnetic interactions are accounted for by the Principle of Minimal Electromagnetic Coupling. This is to replace $\mathbf{p}$ by $\mathbf{p} - \frac{q}{c}\mathbf{A}$ in the Hamiltonian. Opening up $(\mathbf{p} - \frac{q}{c}\mathbf{A})^2$ leads to four terms. Two of them, $\mathbf{p} \cdot \mathbf{p}$ and $\mathbf{A} \cdot \mathbf{A}$, are handled as described above in Eqs. (20) and (24). The remaining two terms are cross terms of the form $\mathbf{p} \cdot \mathbf{A}$ and $\mathbf{A} \cdot \mathbf{p}$. We will derive an expression for $\nabla \cdot \mathbf{A}$. The expression for $\mathbf{A} \cdot \nabla$ will be its transpose. These expressions must be multiplied by $\left(\frac{1}{2m} \times \frac{\hbar}{i} \times \frac{-q}{c}\right)^*$ and $\left(\frac{1}{2m} \times \frac{\hbar}{i} \times \frac{-q}{c}\right)$ before being placed into the appropriate matrix elements of the magnetic matrix.

The expression that must be computed is

$$\int (\nabla\psi_{19})^* \cdot (\mathbf{A}\psi_{19})\; dx \wedge dy \tag{26}$$

In order to evaluate the first term on the left we use the results in Eq. (22):

$$(\nabla\psi_{19})^* = \begin{bmatrix} \partial\psi/\partial x & \partial\psi/\partial y \end{bmatrix}^* = \begin{bmatrix} \psi_9 - \psi_3 & \psi_5 - \psi_3 \end{bmatrix}^* (J^{-1})^t \tag{27}$$

If we write $(J^{-1})t = \begin{bmatrix} A & B \\ C & D \end{bmatrix}$ then the expression on the right of this equation can be expressed as

$$\begin{bmatrix} \psi_3 & \psi_9 & \psi_5 \end{bmatrix}^* \begin{bmatrix} -A-C & -B-D \\ A & B \\ C & D \end{bmatrix} = \begin{bmatrix} \psi_3 & \psi_9 & \psi_5 \end{bmatrix}^* \left[\begin{array}{cc} * & * \\ \hline & \\ & (J^{-1})^t \\ & \end{array}\right] \tag{28}$$

In this expression the entries * indicate that the choice of this matrix element is such that each column sum is zero. These terms are independent of the coordinate, so may be taken out of the integral.

The right hand side of the integral in Eq. (26) is now

$$\frac{dx \wedge dy}{d\xi \wedge d\eta} \begin{bmatrix} A_{x3}\phi_0 + A_{x9}\phi_1 + A_{x5}\phi_2 \\ A_{y3}\phi_0 + A_{y9}\phi_1 + A_{y5}\phi_2 \end{bmatrix} \times (\psi_3\phi_0 + \psi_9\phi_1 + \psi_5\phi_2)\; d\xi \wedge d\eta \tag{29}$$

The integrals involve only pairwise products of the basis functions ϕ_i, so all are represented by the matrix M_{ij} in Eq.(15). When these results are collected we find the following bilinear expression in the amplitudes ψ^* and ψ:

$$\begin{bmatrix} \psi_3 & \psi_9 & \psi_5 \end{bmatrix}^* |J| \left[\begin{array}{cc} * & * \\ \hline & \\ & (J^{-1})^t \\ & \end{array}\right] \begin{bmatrix} A_{x3} & A_{x9} & A_{x5} \\ A_{y3} & A_{y9} & A_{y5} \end{bmatrix} \frac{1}{24} \begin{bmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{bmatrix} \begin{bmatrix} \psi_3 \\ \psi_9 \\ \psi_5 \end{bmatrix} \tag{30}$$

The matrix elements of the 3×3 matrix must be multiplied by $-(\hbar/i)^*(q/2mc)$ and then placed into the appropriate spots of the $N_V \times N_V$ magnetic matrix.

The matrix elements of $\mathbf{A} \cdot \nabla$ are obtained from the transpose of the 3×3 matrix in Eq. (30):

$$\left[\begin{array}{ccc} \psi_3 & \psi_9 & \psi_5 \end{array} \right]^* |J| \frac{1}{24} \left[\begin{array}{ccc} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{array} \right] \left[\begin{array}{cc} A_{x3} & A_{y3} \\ A_{x9} & A_{y9} \\ A_{x5} & A_{y5} \end{array} \right] \left[\begin{array}{c|c|c} * & & \\ & (J^{-1}) & \\ * & & \end{array} \right] \left[\begin{array}{c} \psi_3 \\ \psi_9 \\ \psi_5 \end{array} \right] \tag{31}$$

This must be multiplied by $-(\hbar/i)(q/2mc)$ and then placed into the appropriate spots of the $N_V \times N_V$ magnetic matrix. The resulting magnetic matrix is hermitian: it is an imaginary antisymmetric matrix.

4.6 Implementing the Details

Introduce the potential $V(x, y)$ and decide on the region of the plane which is of interest. Tesselate this region with vertices and number the vertices from 1 to N_V. Store information about the x and y coordinates of each vertex. Evaluate and store the value of the potential at each vertex. Number the 2-dimensional elements (simplices, or triangles) from 1 to N_E. For each element, identify the three vertices at the "corners".

Create three $N_V \times N_V$ matrices: an overlap matrix, a potential energy matrix, and a kinetic energy matrix. Zero out each.

Scan through the elements from the first $\alpha = 1$ to the last $\alpha = N_E$. For each element (e.g., $\alpha = 19$) determine its three vertices (e.g., $i = 3, 9, 5$). For these three vertices compute 3×3 matrices

Overlap Integral: Eq.(20).

Potential Energy: Eq.(24).

Kinetic Energy: Eq.(28).

Magnetic Energy: Eq.(30).

Add the 9 matrix elements from Eq.(20) into the appropriate places of the $N_V \times N_V$ overlap matrix. Do the same for the other three matrices from Eq.(24) and Eq.(28). The resulting quadratic form in the unknown amplitudes must be stationary to satisfy the variational principle. This means that the generalized eigenvalue equation

$$\langle i|(KE + PE + ME - E)|j\rangle\langle j|\psi\rangle = (\mathcal{H} - E)_{ij}\psi_j = 0 \tag{32}$$

must be solved. Here $\langle i|*|j\rangle$ are the matrix elements of the kinetic energy, potential energy, magnetic energy and overlap matrices, respectively, and the row and column indices identify nodes.

As usual, the results should be sorted by energy, tested for convergence, and then plotted.

Remark: We should open the possibility of computing matrices for terms of the form $\mathbf{p} \cdot \mathbf{A} + \mathbf{A} \cdot \mathbf{p}$ because it is likely to be impossible to coax Matlab to do such calculations for us. These are the interesting type that involve magnetic fields.

5 Matrix Variational Problem

The variational problem of Eq.(1) has now been expressed in matrix form as follows:

$$\delta\left(\psi_i(\mathcal{H}-E)_{ij}\psi_j\right)=0\Rightarrow(\mathcal{H}-E)_{ij}\psi_j=0 \tag{33}$$

The variational equation leads directly and immediately to a matrix eigenvalue equation. Since the "diagonal matrix" $\langle i|E|j\rangle$ is not diagonal, this is a "generalized eigenvalue problem."

5.1 Boundary Conditions

The general boundary condition for bound states is that the wavefunction must be square integrable. This means that the square of the wavefunction must go zero more quickly than $1/r^{D-1}$, where D is the dimension of the problem.

5.1.1 Unbounded Domain

To check whether any of the solutions might be considered of any value, it is useful to make the following test. Divide the vertices up into two subsets: the internal vertices, labeled with indices $r, s, ..$ and the vertices on the boundary, labeled with indices $\beta, \kappa, ...$ Check the ratio

$$\sum_\beta |\psi_\beta|^2 / \sum_r |\psi_r|^2 \tag{34}$$

If this ratio is not small the wavefunction is meaningless. If the ratio is very small the wavefunction might carry physical meaning.

5.1.2 Bounded Domain

In this case the variational problme takes the form

$$\delta\left(\psi_r(\mathcal{H}-E)_{rs}\psi_s+\psi_r(\mathcal{H}-E)_{r\kappa}\psi_\kappa+\psi_\beta(\mathcal{H}-E)_{\beta s}\psi_s+\psi_\beta(\mathcal{H}-E)_{\beta\kappa}\psi_\kappa\right)=0 \tag{35}$$

If the potential is infinite outside the domain of interest, the wavefunction vanishes on the boundary. It is necessary to set all components $\psi_\beta, \psi_\kappa = 0$. As a result the last three terms in the expression above vanish, and the variation must be done only over the values of the wavefucntion at the interior nodes.

5.1.3 Poisson's Equation

In some cases it is necessary to solve Poisson's Equation

$$\nabla^2\Phi=-4\pi\rho \tag{36}$$

where Φ is an unknown electrostatic potential and ρ is a known charge distribution. The finite element is easily modified to treat this problem. The "kinetic energy" matrix for Φ is evaluated as described above. The "diagonal" matrix for ρ is also evaluated (it is the overlap matrix). This leads to the algebraic equation

$$\left(\nabla^2\right)_{ij}\Phi_j=-4\pi\rho_i \tag{37}$$

Now a matrix inversion is called for, rather than a matrix diagonalization.

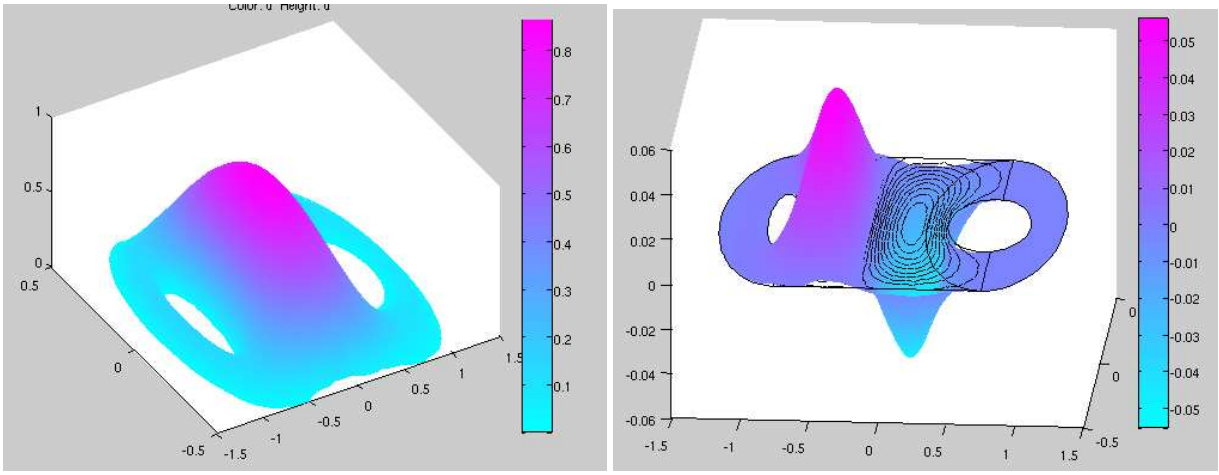

Figure 3: (a) The ground state and (b) first excited state wavefunction for a particle trapped in an infinitely deep potential well whose shape is shown in Fig. 2b.

5.2 Results

The eigenstates for the infinitely deep potential well shown in Fig. 2b were computed using the tesselation shown there. This involved solving a "large" matrix, of order 1000×1000. Modern eigensolvers for sparse matrices made quick work of this. The eigenvectors with the two lowest eigenvalues are shown in Fig. 3. The ground state (Fig. 3a) exhibits no nodes, while the first excited state (Fig. 3b) has a single nodal line that divides the region with the two elliptical holes. The second excited state (not shown) also has one nodal line that passes through both elliptical holes.

It is very clear that an attempt to construct these wavefunctions by analytic means would be extremely frustrating.

6 3D: Linear Functions

In three dimensions the tesselation is in terms of simplices that are conveniently taken as tetrahedra. These have 4 vertices, 6 edges, and 4 faces. The analog of the fundamental right triangle is the right simplex with coordinates: $(0,0,0) \to 0, (1,0,0) \to 1, (0,1,0) \to 2, (0,0,1) \to 3$.

6.1 Linear Basis Functions

The analog of Eq.(??) is

$$\begin{array}{rcl} \phi_0(\xi,\eta,\zeta) &=& 1-\xi-\eta-\zeta \\ \phi_1(\xi,\eta,\zeta) &=& \xi \\ \phi_2(\xi,\eta,\zeta) &=& \eta \\ \phi_3(\xi,\eta,\zeta) &=& \zeta \end{array} \tag{38}$$

6.2 Integrals

The analogs of Eqs.(22,26) for linear functions in 3D is

$$\begin{array}{lcl} (2) & = & 1/60 \\ (1,1) & = & 1/120 \end{array} \qquad \begin{array}{lcll} (3) & = & 1/120 & = & 6/720 \\ (2,1) & = & 1/360 & = & 2/720 \\ (1,1,1) & = & 1/720 & = & 1/720 \end{array} \tag{39}$$

6.3 Overlap Matrix

If the real-space simplex has vertices numbered 3, 9, 5, 7, the analog of Eq.(23) is:

$$\frac{1}{120} \left| \begin{array}{ccc} x_9 - x_3 & y_9 - y_3 & z_9 - z_3 \\ x_5 - x_3 & y_5 - y_3 & z_5 - z_3 \\ x_7 - x_3 & y_7 - y_3 & z_7 - z_3 \end{array} \right| \times \left[\begin{array}{cccc} \psi_3 & \psi_9 & \psi_5 & \psi_7 \end{array} \right] \left[\begin{array}{cccc} 2 & 1 & 1 & 1 \\ 1 & 2 & 1 & 1 \\ 1 & 1 & 2 & 1 \\ 1 & 1 & 1 & 2 \end{array} \right] \left[\begin{array}{c} \psi_3 \\ \psi_9 \\ \psi_5 \\ \psi_7 \end{array} \right] \tag{40}$$

The absolute value of the jacobian should be taken. It remains to place the 16 numbers that occur in this 4×4 matrix onto the right places in the large $N_V \times N_V$ matrix representing $\int\int \psi^*(x,y,z)\, E\, \psi(x,y,z)\, dx\wedge dy \wedge dz$.

6.4 Potential Energy Matrix

This matrix is computed following the rules laid out in Sect. 3.3. The result involves

a prefactor: $\frac{1}{720}$ in 3D as compared with $\frac{1}{120}$ in 2D.

a jacobian: as given in Eq.() above, as opposed to the 2×2 matrix given in Eq.().

column and row vectors: the four component matrices as given in Eq.() above, as opposed to those with 3 given in Eq.().

a 4×4 matrix: this is the interesting part:

$$\left[\begin{array}{cccc} 6V_3 + 2V_9 + 2V_5 + 2V_7 & 2V_3 + 2V_9 + 1V_5 + 1V_7 & 2V_3 + 1V_9 + 2V_5 + 1V_7 & 2V_3 + 1V_9 + 1V_5 + 2V_7 \\ 2V_3 + 2V_9 + 1V_5 + 1V_7 & 2V_3 + 6V_9 + 2V_5 + 2V_7 & 1V_3 + 2V_9 + 2V_5 + 1V_7 & 1V_3 + 1V_9 + 2V_5 + 2V_7 \\ 2V_3 + 1V_9 + 2V_5 + 1V_7 & 1V_3 + 2V_9 + 2V_5 + 1V_7 & 2V_3 + 2V_9 + 6V_5 + 2V_7 & 1V_3 + 1V_9 + 2V_5 + 2V_7 \\ 2V_3 + 1V_9 + 1V_5 + 2V_7 & 1V_3 + 2V_9 + 1V_5 + 2V_7 & 1V_3 + 1V_9 + 2V_5 + 2V_7 & 2V_3 + 2V_9 + 2V_5 + 6V_7 \end{array} \right] \tag{41}$$

This expression can be simplified by representing each matrix element as the inner product between a row vector of integer coefficients and a column vector of values of the potential at the appropriate vertices: e.g., the (1,2) matrix element is $(2,2,1,1) \times (V_3, V_9, V_5, V_7)^t$. The matrix above is written in simpler form as

$$\left[\begin{array}{cccc} (6,2,2,2) & (2,2,1,1) & (2,1,2,1) & (2,1,1,2) \\ (2,2,1,1) & (2,6,2,2) & (1,2,2,1) & (1,1,2,2) \\ (2,1,2,1) & (1,2,2,1) & (2,2,6,2) & (1,1,2,2) \\ (2,1,1,2) & (1,2,1,2) & (1,1,2,2) & (2,2,2,6) \end{array} \right] \tag{42}$$

We note that the sum of the coefficients (120), divided by the prefactor (720), is $\frac{120}{720} = \frac{1}{3!}$, the volume of the right tetrahedron. Similarly, in 2D: $\frac{60}{120} = \frac{1}{2!}$ is the area of the reference right triangle. This means that the effect of the potential within each simplex is appropriately averaged over the vertices of the simplex.

6.5 Kinetic Energy Matrix

The analog of Eq. (24) is

$$\left[\begin{array}{cccc} \psi_3 & \psi_9 & \psi_5 & \psi_7 \end{array}\right] \left[\begin{array}{c|ccc} * & c_2 & c_3 & c_4 \\ \hline r_2 & & & \\ r_3 & & (JJ^t)^{-1} & \\ r_4 & & & \end{array}\right] \left[\begin{array}{c} \psi_3 \\ \psi_9 \\ \psi_5 \\ \psi_7 \end{array}\right] \tag{43}$$

Here the matrix element r_2 is chosen so that the sum of all the matrix elements in the second row is zero. The matrix elements r_3 and r_4 are chosen so the row sums are zero. Similarly, c_2, c_3, c_4 are chosen so that the column sums (2,3,4) vanish. Finally, * is chosen so that the first row/column sum vanishes.

6.6 Magnetic Matrix

The analog of Eq. (30) is

$$\left[\begin{array}{cccc} \psi_3 & \psi_9 & \psi_5 & \psi_7 \end{array}\right]^* \left[\begin{array}{ccc} * & * & * \\ \hline & (J^{-1})^t & \\ & & \end{array}\right] \left[\begin{array}{cccc} A_{x3} & A_{x9} & A_{x5} & A_{x7} \\ A_{y3} & A_{y9} & A_{y5} & A_{y7} \\ A_{z3} & A_{z9} & A_{z5} & A_{z7} \end{array}\right] \frac{1}{120} \left[\begin{array}{cccc} 2 & 1 & 1 & 1 \\ 1 & 2 & 1 & 1 \\ 1 & 1 & 2 & 1 \\ 1 & 1 & 1 & 2 \end{array}\right] \left[\begin{array}{c} \psi_3 \\ \psi_9 \\ \psi_5 \\ \psi_7 \end{array}\right] \tag{44}$$

6.7 Implementing the Details

Introduce the potential $V(x, y, z)$ and decide on the spacial domain of interest. Tesselate this region with vertices and number the vertices from 1 to N_V. Store information about the x, y, and z coordinates of each vertex. Evaluate and store the value of the potential at each vertex. Number the 3-dimensional elements (simplices, or tetrahedra) from 1 to N_E. For each element, identify the four vertices at the "corners". If the mass is not the same for all elements, provide mass information for each element.

Create four $N_V \times N_V$ matrices: an overlap matrix, a potential energy matrix, a kinetic energy matrix, and a "magnetic matrix". Zero out each.

Scan through the elements from the first $\alpha = 1$ to the last $\alpha = N_E$. For each element (e.g., $\alpha = 19$) determine its four vertices (e.g., $i = 3, 9, 5, 7$). For these four vertices compute 4×4 matrices

Overlap Integral: Eq.(40).

Potential Energy: Eq.(41).

Kinetic Energy: Eq.(43).

Magnetic Matrix: Eq.(44).

Add the 16 matrix elements from Eq.(XX) into the appropriate places of the $N_V \times N_V$ overlap matrix. Do the same for the other three matrices from Eq.(24), Eq.(XX), and Eq.(28). The resulting quadratic form in the unknown amplitudes must be stationary to satisfy the variational principle. This means that the generalized eigenvalue equation

$$\langle i|(KE + PE + ME - E)|j\rangle\langle j|\psi\rangle = 0 \tag{45}$$

must be solved. Here $\langle i|*|j\rangle$ are the matrix elements of the kinetic energy, potential energy, magnetic energy, and overlap matrices, respectively, and the row and column indices identify nodes.

7 Quantum Mechanics in the Finite Element Representation

We have computed energy eigenvalues and wavefunctions using the finite element method. This method is used to transform differential equations to matrix equations. In a sense this method can be regarded as a change of basis procedure similar in spirit to the standard (Dirac) transformation theory for Quantum Mechanics. As a result we can ask the usual basic questions: What are the basis functions? What is the matrix representative of the position operator? The momentum operator? Are commutation relations preserved? Is the matrix representative of x^2 equal to the square of the matrix representative of x?

7.1 Basis Functions

The matrix elements of all the matrices constructed so far are indexed by an integer i, where i labels the various vertices in the tesselation. We define a set of "basis" functions for our matrix representation by $|i\rangle$, with a $1:1$ correspondence between the vertices i and the basis functions $|i\rangle$. In the coordinate representation these functions are $\langle x|i\rangle$. These functions assume value 1 at vertex i and fall off linearly to zero at the other two vertices of each of the triangles sharing i as a vertex.

This set of N_v functions is nonorthogonal and incomplete. They cannot form a basis in the usual sense. They do form a basis set for the piecewise linear functions that are defined by their values at the vertices i. These functions are continuous everywhere, linear in the interior of each element, and not differentiable on the boundaries of the elements. When we call these functions basis functions we mean specifically within the space of such linear functions.

Dirac's representation of Quantum Theory uses orthonormal and complete sets of basis functions. The FEM representation therefore shares some of the properties of Dirac's more familiar formulation, and lacks some of the others.

The most important function that we can construct from these functions is the matrix of overlap integrals

$$\mathcal{O}_{ij} = \langle i|j\rangle = \int \langle i|x\rangle \; dx \; \langle x|j\rangle = G_{ij} \tag{46}$$

where $\langle i|x\rangle = \langle x|i\rangle^*$ and G_{ij} reminds us that these overlap integrals should be considered as the matrix elements of a metric tensor. The metric tensor is nonsingular, sparse, and real if the functions $\langle x|j\rangle$ are real.

It is very useful to introduce an alternate basis defined by

$$|\tilde{r}\rangle = |i\rangle(G^{-1/2})_{ir} \tag{47}$$

Although the metric tensor G is sparse its inverse G^{-1} is not; nor is $G^{-1/2}$. This means that the corresponding spatial basis states $\langle x|\tilde{r}\rangle = \langle x|i\rangle(G^{-1/2})_{ir}$ are not nearly as localized as the original basis functions $\langle x|i\rangle$. **We should create a picture to illustrate this.**

These N_v new basis vectors are orthonormal:

$$\langle\tilde{r}|\tilde{s}\rangle = (G^{-1/2})_{ri}\langle i|j\rangle(G^{-1/2})_{js} = (G^{-1/2})_{ri}G_{ij}(G^{-1/2})_{js} = \delta_{rs} \tag{48}$$

The resolution of the identity is simple in terms of the new set of vectors:

$$I = |\tilde{r}\rangle\langle\tilde{r}| \rightarrow |i\rangle(G^{-1/2})_{ir}(G^{-1/2})_{rj}\langle j| = |i\rangle(G^{-1})_{ij}\langle j| \tag{49}$$

It is possible to find two matrix representations of an operator $\hat{A}$: one in the original basis and one in the orthonormal basis. These are related by

$$\langle\tilde{r}|\hat{A}|\tilde{s}\rangle = (G^{-1/2})_{ri}\langle i|\hat{A}|j\rangle(G^{-1/2})_{js} \qquad \text{or} \qquad \tilde{A} = G^{-1/2}AG^{-1/2} \tag{50}$$

The operator A can be reconstructed from its matrix elements. Starting from the orthonormal set, we have

$$A = |\tilde{r}\rangle\tilde{A}_{rs}\langle\tilde{s}| = |i\rangle(G^{-1/2})_{ir}(G^{-1/2})_{rk}A_{kl}(G^{-1/2})_{ls}(G^{-1/2})_{sj}\langle j| = |i\rangle(G^{-1}AG^{-1})_{ij}\langle j| \tag{51}$$

Operator products are constructed as follows

$$\tilde{AB} = \langle\tilde{r}|AB|\tilde{t}\rangle = \langle\tilde{r}|A|\tilde{s}\rangle\langle\tilde{s}|B|\tilde{t}\rangle = \tilde{A}\tilde{B} = \left(G^{-1/2}AG^{-1/2}\right)\left(G^{-1/2}BG^{-1/2}\right) = G^{-1/2}AG^{-1}BG^{-1/2} \tag{52}$$

In a similar way the operator product $\hat{AB}$ can be expressed as follows:

$$\hat{AB} = |i\rangle(G^{-1}AG^{-1}BG^{-1})_{ij}\langle j| \tag{53}$$

Here the matrices A and B sandwiched between the G^{-1} are the matrices of the operators $\hat{A}$ and $\hat{B}$ with respect to the original nonorthogonal basis vectors.

The prescription for finding the matrix representation of an operator $\hat{A}$ is therefore:

1. Compute the matrix elements of the operator in the original basis.
2. Multiply on both sides by G^{-1}.
3. $\hat{A} = |i\rangle(G^{-1}AG^{-1})_{ij}\langle j|$

It remains to see how good an approximation this is to the operator A. For example, is the matrix representation of x^2 well approximated by the suitable square of the matrix representation of the operator x?

With these remarks in hand we turn now to the computation of the matrices representing several important operators. These matrices will be computed with respect to the nonorthogonal basis set. These can be transformed to the matrices with respect to the orthonormal basis set as shown in Eq. (50).

7.2 The Position Operator in the Linear FEM Basis

The matrix representation of the x coordinate of the position operator is built up in the usual fashion by carrying out the integral $\int \psi_{19} x \psi_{19} dx \wedge dy$. We first express the x coordinate in terms of the coordinates of points 3, 9, 5:

$$x = x_3 + (x_9 - x_3)\xi + (x_5 - x_3)\eta = x_3\phi_0 + x_9\phi_1 + x_5\phi_2 \tag{54}$$

The integral over this triangle is

$$|J| \int\int (\psi_3\phi_0 + \psi_9\phi_1 + \psi_5\phi_2)^2 (x_3\phi_0 + x_9\phi_1 + x_5\phi_2)\ d\xi \wedge d\eta \tag{55}$$

It is clear that the result involves integrals over products of three linear basis functions, which are given in Eq. (18). In fact, the result is evident by making a small change in Eq. (20):

$$\frac{|J|}{120} \begin{vmatrix} x_9 - x_3 & y_9 - y_3 \\ x_5 - x_3 & y_5 - y_3 \end{vmatrix} \times \begin{bmatrix} \psi_3 & \psi_9 & \psi_5 \end{bmatrix} \begin{bmatrix} 6x_3 + 2x_9 + 2x_5 & 2x_3 + 2x_9 + 1x_5 & 2x_3 + 1x_9 + 2x_5 \\ 2x_3 + 2x_9 + 1x_5 & 2x_3 + 6x_9 + 2x_5 & 1x_3 + 2x_9 + 2x_5 \\ 2x_3 + 1x_9 + 2x_5 & 1x_3 + 2x_9 + 2x_5 & 2x_3 + 2x_9 + 6x_5 \end{bmatrix} \begin{bmatrix} \psi_3 \\ \psi_9 \\ \psi_5 \end{bmatrix} \tag{56}$$

It should be pointed out that the matrix representation of the first cordinate of the position operator $\mathbf{x} = (x_1, x_2) = (x, y)$ depends on the y coordinates of the vertices in the tesselation through the value of the jacobian. Similar results hold for the matrix representation of the y coordinate. In the event that the tesselation is regular (all simplices have the same measure) the matrix representation of the first coordinate x is independent of all y coordinates.

If it is necessary to use complex wavefunctions, the row vector on the left should be conjugated. Extensions to 3 dimensions are straightforward.

7.3 The Momentum Operator in the Linear FEM Basis

We compute the matrix representation of the gradient operator:

$$\int \psi_{19}^* \begin{bmatrix} \partial/\partial x \\ \partial/\partial y \end{bmatrix} \psi_{19}\ dx \wedge dy = |J| \int (\psi_3\phi_0 + \psi_9\phi_1 + \psi_5\phi_2)^* J^{-1} \begin{bmatrix} \psi_9 - \psi_3 \\ \psi_5 - \psi_3 \end{bmatrix} d\xi \wedge d\eta \tag{57}$$

We have used Eq. (22) to replace the action of the partial derivatives on the wavefunction by a column vector of differences. The integral is linear in the basis functions. Further, $\int\int \phi_i(\xi, \eta) d\xi \wedge d\eta = \frac{1}{6}$ for each of the basis functions. Putting this all together, we find

$$\int \psi_{19}^* \begin{bmatrix} \partial/\partial x \\ \partial/\partial y \end{bmatrix} \psi_{19}\ dx \wedge dy = |J|\ \frac{1}{6}(\psi_3 + \psi_9 + \psi_5)^* \left[\begin{array}{c|c} * & \\ & J^{-1} \\ * & \end{array}\right] \begin{bmatrix} \psi_3 \\ \psi_9 \\ \psi_5 \end{bmatrix} \tag{58}$$

As before, the matrix elements * are chosen so that the row sums vanish.

XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX?? remove

7.4 Function Algebra

The basis functions $|\phi_i\rangle$ can be used to represent functions that have known values at each vertex: $f(x) \to \sum f_i \phi_i(x)$. Such functions form a linear vector space, and the functions $\phi_i(x)$ are a basis

set for the linear vector space of functions that are linear on each element. The column vectors $col(f_i)$ represent these functions. Addition is simple: $\alpha f(x) + \beta g(x) \to col(\alpha f_i + \beta g_i)$. However, these vectors cannot be used to describe the composition properties $f \times g$ under multiplication.

To get around this problem we map each function to an operator: an $N_v \times N_v$ diagonal matrix under

$$f(x) \to \sum f_i \phi_i(x) \to col(f_i) \to \hat{f} \to \sum |\tilde{r}\rangle f_r \langle \tilde{r}| \tag{59}$$

This is a diagonal matrix. Addition and multiplication are well-defined: $\alpha f \hat{+} \beta g = \alpha \hat{f} + \beta \hat{g}$ and $(f \hat{*} g) = \hat{f} \times \hat{g}$. The matrix elements of the diagonal matrix representation of f are

$$\langle i|\hat{f}|j\rangle = \langle i|\hat{r}\rangle f_r \langle \hat{r}|j\rangle = (G^{1/2})_{ir} f_r (G^{1/2})_{rj} \tag{60}$$

7.5 Operator Algebra

Suppose that we have two operators A and B. To construct a matrix representation of these operators with nice algebraic properties, we should be able to construct operators representing their sum and their product from the matrix representations of the operators themselves.

Define $\Gamma(A)$ to be the matrix representing the operator A in some finite element construction (i.e., a tesselation is specified, followed by specification of basis functions). Similarly: $B \to \Gamma(B)$.

It is intuitive that $\Gamma(A+B) = \Gamma(A) + \Gamma(B)$; it is even easy to prove. It is not intuitive, even not correct, that $\Gamma(A \cdot B) = \Gamma(A) \times \Gamma(B)$, where $\cdot$ means operator product and $\times$ is matrix multiplication.

Is there some way we can turn operator products into matrix multiplication of some type? To get a sense of this, set $B = I$, where I is the identity operator. Then define

$$\Gamma(A) = \Gamma(A \cdot I) = \Gamma(A) \otimes \Gamma(I) = \Gamma(A) \tag{61}$$

In this expression $\Gamma(I) = \mathcal{O}$ is the matrix of overlap integrals. If Eq. (51) is to be true as an identity, then $\otimes = \mathcal{O}^{-1}$. Elegantly: $\Gamma(\cdot) = \mathcal{O}^{-1} = \Gamma^{-1}(I)$. The conclusion is that we can represent operator products as matrix products by inserting the inverse of the overlap matrix between each of the operators that we are taking the product of:

$$\Gamma(A \cdot B) = \Gamma(A) \times \Gamma(\cdot) \times \Gamma(B) = \Gamma(A) \times \mathcal{O}^{-1} \times \Gamma(B) \tag{62}$$

In particular

$$\Gamma(KE) = \frac{\hbar^2}{2m} \Gamma(\nabla)^* \times \mathcal{O}^{-1} \times \Gamma(\nabla) \tag{63}$$

It is necessary to check these assertions!!

xXXXXXXXXXXXXXXXXXXX ??? remove

7.6 Measure

Remark: One natural question that may come up is: What measure should we assign to each vertex? In the natural linear basis, I have good arguments for the following response. Compute M, the area/volume (measure) of the physical space that is being approximated. Determine the trace of the overlap matrix computed before boundary conditions are applied: $T = \sum_{i=1}^{N_V} OL_{ii}$. The measure associated with vertex i is $\mu(i) = OL_{ii} \times (M/T)$. We need a 'proof by picture'.

Table 1: In 2 dimensions the size of the basis function set over simplices with 3 vertices grows with the number of degrees of freedom. The number of independent monomials of degree 0, 1, 2, 3, 4, 5 as well as the minimum appropriate number (total) is shown. The number of "extra" functions is the kernel of the matrix of function values.

Continuity	Partials	d.o.f./vertex	d.o.f./element	total	0	1	2	3	4	5	d.kernel
C^0	ψ	1	$1 \times 3 = 3 =$	$3 =$	1	2					0
C^1	$\partial\psi$	$1 + 2$	$3 \times 3 = 9 <$	$10 =$	1	2	3	4			1
C^2	$\partial^2\psi$	$1 + 2 + 3$	$6 \times 3 = 18 <$	$21 =$	1	2	3	4	5	6	3

8 Degrees of Freedom

Sometimes some of the tacit assumptions underlying these calculations must be relaxed. These assumptions include:

1. Only a finite domain in needs to be considered.
2. Only bound states are of interest.
3. Only continuity of the wavefunction needs to be considered.

There is a solution for each of these problems. In this section we treat only the third assumption. We do this in almost the weakest possible way. We show how to enforce continuity of the first derivatives of the wavefunction in two dimensions.

To this end, we introduce *three* unknown amplitudes at each vertex. There are

$$\psi_{i,0} = \psi|_i \qquad \psi_{i,1} = \frac{\partial\psi}{\partial x}|_i \qquad \psi_{i,2} = \frac{\partial\psi}{\partial y}|_i \tag{64}$$

If we wanted also continuity of the second derivatives we would have to introduce three additional degrees of freedom at each vertex.

Now the set of basis functions in each element consists of $9 = 3 \times 3$ functions. The first factor of 3 comes from having 3 vertices for each element; the second factor of 3 comes from having one scalar value and two first partial derivatives to estimate at each vertex.

As before, computations are carried out by linearly mapping each simplex into a benchmark triangle and carrying out the computations there. The basis functions need to be computed on the benchmark triangle, and the derivatives and integrals carried out there. The 9 basis functions will be constructed from the monomials in ξ and η of the lowest possible degree. The number of monomials of degree 0, 1, 2, 3,... is 1, 2, 3, 4, ... and the cumulative number of terms is 1, 3, 6, 10, ... Therefore it suffices to use up to cubic terms, there are 10 of them, to construct the 9 independent — but nonorthogonal — basis functions on the benchmark triangle. The cost for imposing C^2 continuity can also be computed. These costs are summarized in Table 1 for tesselations in 2D. Table 2 is the extension of Table 1 for three dimensional cases.

8.1 Warm Up Example

In order to ease into this algorithmic process for computing basis functions we will compute the three functions $\phi_i(\xi, \eta)$, $i = 0, 1, 2$, that were used in Section 3. Define a linear combination: $\phi_0 =$

Table 2: In 3 dimensions the size of the basis function set over simplices with 4 vertices grows with the number of degrees of freedom. The number of independent monomials of degree 0, 1, 2, 3, 4, 5 as well as the minimum appropriate number (total) is shown. The number of "extra" functions is the kernel of the matrix of function values.

Continuity	Partials	d.o.f./vertex	d.o.f./element	total	0	1	2	3	4	5	d.kernel
C^0	ψ	1	$1 \times 4 = 4 =$	$4 =$	1	3					0
C^1	$\partial\psi$	$1+3$	$4 \times 4 = 16 <$	$20 =$	1	3	6	10			4
C^2	$\partial^2\psi$	$1+3+6$	$10 \times 4 = 40 <$	$56 =$	1	3	6	10	15	21	16

$a_1 + a_2\xi + a_3\eta$ that is 1 on vertex $(\xi, \eta) = (0, 0)$ and zero on the other two vertices; $\phi_1 = b_1 + b_2\xi + b_3\eta$ that is 1 on vertex $(1, 0)$ and zero on the other two vertices; and $\phi_2 = c_1 + c_2\xi + c_3\eta$ that is 1 on vertex $(0, 1)$ and zero on the other two vertices. These coefficients can be organized systematically into matrix form:

$$\begin{bmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix} \begin{bmatrix} a_1 & b_1 & c_1 \\ a_2 & b_2 & c_2 \\ a_3 & b_3 & c_3 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{65}$$

The first matrix contains information about the values of the functions at the various vertices. For example, the third row provides the values of the three functions: $1, \xi, \eta$ at the third point $2 = (0, 1)$. The second matrix contains the three sets of unknown coefficients for the three desired functions, organized as column vectors. The matrix on the right shows that the first function (defined by the as) is 1 at the first point $(0, 0)$ and zero at the second $(1, 0)$ and third $(0, 1)$ points. This information is contained in the first column (c.f., Eq.(14)). The coefficients are given by the inverse of the left-most matrix:

$$\begin{bmatrix} a_1 & b_1 & c_1 \\ a_2 & b_2 & c_2 \\ a_3 & b_3 & c_3 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix}^{-1} = \begin{bmatrix} 1 & 0 & 0 \\ -1 & 1 & 0 \\ -1 & 0 & 1 \end{bmatrix} \tag{66}$$

Each column in the resulting inverse matrix provides the coefficients for one of the desired basis functions (c.f., Eq.(13)). For example, the three coefficients in the first column $(+1, -1, -1)$ tell us that $\phi_0(\xi, \eta) = 1 - \xi - \eta$.

8.2 Cubic Functions for C^1 Continuity

We now return to the problem of constructing a set of basis functions that ensure continuity of the wavefunction and its first derivatives at the vertices of a simplex. The basis functions are constructed by taking a linear combination of the 9 monomials $\xi^p\eta^q$, $p \geq 0, q \geq 0, p + q \leq 3$, and satisfying conditions. To be specific, we write

$$\phi = \left[\begin{array}{c|cc|ccc|cccc} 1 & \xi & \eta & \xi^2 & \xi\eta & \eta^2 & \xi^3 & \xi^2\eta^1 & \xi^1\eta^2 & \eta^3 \end{array}\right] \left[\begin{array}{c} a_{0,0} \\ \hline a_{1,0} \\ a_{0,1} \\ \hline a_{2,0} \\ a_{1,1} \\ a_{0,2} \\ \hline a_{3,0} \\ a_{2,1} \\ a_{1,2} \\ a_{0,3} \end{array}\right] \tag{67}$$

We now apply this equation as follows. We set $(\xi, \eta) = (0, 0)$ and demand that the resulting function is 1 at vertex 0 of the benchmark triangle, zero at the other two vertices, and all derivatives vanish at all vertices. This gives one condition on the coefficients $a_{p,q}$. Now compute $\partial\phi/\partial\xi$ and evaluate it at this point. Require that this function have value 1 at vertex 0 and vanishes everywhere else. Similarly for $\partial\phi/\partial\eta$. This gives a set of three conditions on the coefficients $a_{p,q}$. The first is that the wavefunction itself is 1 at 0 and vanishes at vertices 1 and 2. The second is that its first derivative with respect to ξ is 1 at 0 and vanishes at vertices 1 and 2. The third is that its first derivative with respect to η is 1 at 0 and vanishes at vertices 1 and 2. This triplet of conditions is repeated at vertices $1 = (1, 0)$ and $2 = (0, 1)$. The resulting set of 9 equations can be expressed as

$$\begin{array}{cc} & \\ (0,0) & 0 \\ & 1 \\ & 2 \\ & \\ (1,0) & 0 \\ & 1 \\ & 2 \\ & \\ (0,1) & 0 \\ & 1 \\ & 2 \end{array} \left[\begin{array}{c|cc|ccc|ccc|c} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \hline 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \hline 1 & 1 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 2 & 0 & 0 & 3 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 & 0 & 1 & 0 & 0 \\ \hline 1 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 2 & 0 & 0 & 0 & 3 \end{array}\right] \quad [A] = \left[\begin{array}{cccccccccc} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{array}\right] \tag{68}$$

In this equation the first three rows impose conditions at point 0 in the (ξ, η) plane with coordinates $(0, 0)$. The three conditions are: $\psi, \partial\psi/\partial\xi, \partial\psi/\partial\eta$ are 1 and vanish elsewhere. The second and third triplet of rows impose the same conditions, but at vertices $1 = (1, 0)$ and $2 = (0, 1)$.

The matrix $[A]$ is a 10×9 matrix. The first column gives the 10 coefficients $a_{p,q}$ of the function ϕ which is 1 at $(0, 0)$, which vanishes at the other two points, and whose ξ and η derivatives are zero at all three points. The second column defines the function ϕ for which $\partial\phi/\partial\xi$ is 1 at $(0, 0)$, but whose values and derivatives are 0 elsewhere. The remaining columns provide analogous information.

The columns define the basis functions, but there is a small problem. It's not easy to invert a 9×10 matrix. To get around this minor problem, we compute the *kernel* of the matrix on the left. This is a vector that is orthogonal to all the nine rows in this matrix. The kernel consists of one vector with 10 components. It is unique up to sign and scale. It is convenient to take this as the vector $[0, 0, 0, 0, -1, 0, 0, 1, 1, 0]$. If we adjoin this row vector to the bottom of the 9×10 matrix on the left hand side of Eq.(34) we have a nonsingular 10×10 matrix. The matrix on the right must also be completed to a 10×10 matrix. This can be done in two ways. (i) A row of zeros can be adjoined. In this case $\phi_{10}(\xi, \eta)$ is identically zero. (ii) It can be completed to a 10×10 identity matrix. In this case $\phi_{10}(\xi, \eta)$ is a nontrivial function whose values and first derivates vanish at all

three vertices. As a next step the 10×10 matrix of coefficients $[A]$ is solved for by matrix inversion. The three sets of three columns of $[A]$ define functions ϕ with special properties at the three points 0, 1, 2. This matrix is

$$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -3 & -2 & 0 & 3 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1/3 & -1/3 & 0 & 0 & 1/3 & 0 & 1/3 & 0 & -1/3 \\ -3 & 0 & -2 & 0 & 0 & 0 & 3 & 0 & -1 & 0 \\ 2 & 1 & 0 & -2 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1/3 & -2/3 & 0 & 0 & 2/3 & 0 & -1/3 & 0 & 1/3 \\ 0 & -2/3 & 1/3 & 0 & 0 & -1/3 & 0 & 2/3 & 0 & 1/3 \\ 2 & 0 & 1 & 0 & 0 & 0 & -2 & 0 & 1 & 0 \end{bmatrix} \tag{69}$$

from which it is an easy matter to read off the nine basis functions for the benchmark triangle. They are:

$$\begin{array}{rclcl} \phi_1 &=& 1 - 3\xi^2 - 3\eta^2 + 2\xi^3 + 2\eta^3 & & \\ \phi_2 &=& \xi - 2\xi^2 + \xi^3 + \frac{1}{3}(-\xi\eta + \xi^2\eta - 2\xi\eta^2) &=& \xi - 2\xi^2 + \xi^3 - \xi\eta^2 + \phi_{10} \\ \phi_3 &=& \eta - 2\eta^2 + \eta^3 + \frac{1}{3}(-\xi\eta + \xi\eta^2 - 2\xi^2\eta) &=& \eta - 2\eta^2 + \eta^3 - \eta\xi^2 + \phi_{10} \\ \phi_4 &=& 3\xi^2 - 2\xi^3 & & \\ \phi_5 &=& -\xi^2 + \xi^3 & & \\ \phi_6 &=& \frac{1}{3}(\xi\eta + 2\xi^2\eta - \xi\eta^2) &=& \xi^2\eta - \phi_{10} \\ \phi_7 &=& 3\eta^2 - 2\eta^3 & & \\ \phi_8 &=& \frac{1}{3}(\xi\eta + 2\xi\eta^2 - \xi^2\eta) &=& \eta^2\xi - \phi_{10} \\ \phi_9 &=& -\eta^2 + \eta^3 & & \\ & & & & \\ \phi_{10} &=& \frac{1}{3}(-\xi\eta + \xi\eta^2 + \xi^2\eta) & & \end{array} \tag{70}$$

8.3 "Gauge" Freedom

The shape function ϕ_{10}, as well as its derivatives with respect to both ξ and η, evaluates to 0 on the three vertices. This functions behaves in the spirit of "gauge" transformations. The algebraic expressions for the shape functions can be simplified by adding or subtracting ϕ_{10} to: $\phi_2, \phi_3, \phi_6, \phi_8$. We may/maynot make this transformation in our applications. Such simplification does not change the nature of the symmetries described next.

8.4 Symmetries of the Cubic Functions

These shape functions exhibit the following symmetries under the reflection operation $\mathcal{R}$ that exchanges ξ with η:

$$\begin{array}{cc} & \mathcal{R} \\ \hline \phi_1 & \leftrightarrow \quad \phi_1 \\ \phi_2 & \leftrightarrow \quad \phi_3 \\ \phi_4 & \leftrightarrow \quad \phi_7 \\ \phi_5 & \leftrightarrow \quad \phi_9 \\ \phi_6 & \leftrightarrow \quad \phi_8 \\ \\ \phi_{10} & \leftrightarrow \quad \phi_{10} \end{array} \tag{71}$$

This observation is responsible for a few symmetries in the matrix of overlap integrals, but is much more important in reducing the number of matrix elements in computations of the kinetic energy matrix. For example, to compute the kinetic energy matrix it is necessary to compute gradients of the shape functions. The symmetries describe above lead to the symmetry

$$\mathcal{R}\frac{\partial}{\partial \xi}\ \phi_i = \frac{\partial}{\partial \eta}\ \phi_{\mathcal{R}i} \tag{72}$$

The following relations are useful in reducing the number of independent matrix elements:

$$\begin{array}{rcl} \phi_1 &=& 1-(\phi_4+\phi_7) \\ \phi_2 &=& \xi-(\phi_4+\phi_5)-\phi_8 \\ \phi_3 &=& \eta-(\phi_7+\phi_9)-\phi_6 \end{array} \tag{73}$$

In the construction of the kinetic energy matrix a number of symmetries will occur, as can be seen by inspection:

$$\begin{array}{rcrcl} \partial_\eta\phi_4 &=& \partial_\eta\phi_5 &=& 0 \\ \partial_\xi\phi_7 &=& \partial_\xi\phi_9 &=& 0 \\ \partial_\xi\phi_1 &=& -\partial_\xi\phi_4 & & \\ \partial_\eta\phi_1 &=& -\partial_\eta\phi_7 & & \\ \partial_\eta\phi_2 &=& -\partial_\eta\phi_8 & & \\ \partial_\xi\phi_3 &=& -\partial_\xi\phi_6 & & \end{array} \tag{74}$$

9 2D: Cubic Functions

Next, information about values and derivatives in the physical space is used to determine the approximation to the wavefunction on the benchmark triangle. This is done by setting

$$\psi_{19}(x,y) = \sum_\alpha \sum_i A_{\alpha,i}\phi_{\alpha,i}(\xi,\eta) \tag{75}$$

Here $\alpha = 0,1,2$ indexes the three vertices of the simplex and $i = 0,1,2$ indexes a condition on the basis function: $i = 0$ is the value of the function, $i = 1$ is the value of the first derivative with respect to ξ, and $i = 2$ is the value of the first derivative with respect to η.

With the numbering as before ($3, 9, 5$ for element 19) it is a simple matter to determine $A_{0,0} = \psi_3$, $A_{1,0} = \psi_9$, and $A_{2,0} = \psi_5$. Determining the coefficients for the derivative terms is only slightly more of a problem. Using Eq.(16) we have

$$\left[\begin{array}{c} \partial\phi/\partial\xi \\ \partial\phi/\partial\eta \end{array}\right] = J \left[\begin{array}{c} \partial\psi/\partial x \\ \partial\psi/\partial y \end{array}\right] \qquad \text{or} \qquad \left[\begin{array}{c} \phi_{\alpha,1} \\ \phi_{\alpha,2} \end{array}\right] = J \left[\begin{array}{c} \psi_{\alpha',1} \\ \psi_{\alpha',2} \end{array}\right] \tag{76}$$

Here (α', α) index the vertices of a simplex in real space and the canonical vertices of the benchmark triangle that it is mapped to, to wit: $(3,0),(9,1),(5,2)$. The subscripts $1,2$ on ψ show derivatives with respect to x and y, while those on ϕ indicated they are taken with respect to their natural variables $\xi_1 = \xi,\ \xi_2 = \eta$. Applying these "boundary conditions", the approximate wavefunction on the benchmark triangle is

$$\phi(\xi,\eta) = \psi_3\phi_{0,0}+\psi_9\phi_{1,0}+\psi_5\phi_{2,0}+\begin{pmatrix} \phi_{0,1} & \phi_{0,2} \end{pmatrix} J \begin{bmatrix} \psi_{3,1} \\ \psi_{3,2} \end{bmatrix}+\begin{pmatrix} \phi_{1,1} & \phi_{1,2} \end{pmatrix} J \begin{bmatrix} \psi_{9,1} \\ \psi_{9,2} \end{bmatrix}+\begin{pmatrix} \phi_{2,1} & \phi_{2,2} \end{pmatrix} J \begin{bmatrix} \psi_{5,1} \\ \psi_{5,2} \end{bmatrix} \tag{77}$$

It is useful to simplify this expression by defining

$$\tilde{\psi}_{i,0} = \psi_{i,0} \qquad \begin{bmatrix} \tilde{\psi}_{i,1} \\ \tilde{\psi}_{i,2} \end{bmatrix} = J \begin{bmatrix} \psi_{i,1} \\ \psi_{i,2} \end{bmatrix} \tag{78}$$

With these definitions the wavefunction can be expressed

$$\psi_{19}(x,y) \to \phi(\xi,\eta) = \sum_{\alpha}\sum_{i} \tilde{\psi}_{\alpha',i}\phi_{\alpha,i}(\xi,\eta) \tag{79}$$

Now that the wavefunction has been represented in terms of unknown quantities that we hope to compute, we can proceed by following in the footsteps of the procedures previously provided. Three matrices are set up and zeroed out. They are each $3N_E \times 3N_E$ matrices. They will contain bilinear forms in the triples $\psi_{i,0}, \psi_{i,1}, \psi_{i,2}$ at each vertex i. Computations of overlap integrals, potential energy matrices, and kinetic energy matrices are constructed, element by element, as indicated above.

9.1 Overlap Matrix:

This is computed by plugging the expression for the wavefunction, Eq.(40), into an equation of the form Eq.(18), expanding, and carrying out the indicated integrals. This results in a quadratic form in the unknowns $\tilde{\psi}_{3,i}, \tilde{\psi}_{9,i}, \tilde{\psi}_{5,i}$ that can be represented by a 9×9 matrix. The matrix elements are integrals of the form $\int\int \phi_{\beta,j}\phi_{\alpha,i} d\xi \wedge d\eta$. These need be carried out only once. The remaining parts of this piece of the overlap matrix depends on the matrix J.

This dependence can be unwound by grouping the information at each vertex in a triplet as follows

$$\begin{bmatrix} \tilde{\psi}_{\alpha',0} \\ \tilde{\psi}_{\alpha',1} \\ \tilde{\psi}_{\alpha',2} \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & J \end{bmatrix} \begin{bmatrix} \psi_{\alpha',0} \\ \psi_{\alpha',1} \\ \psi_{\alpha',2} \end{bmatrix} = \mathcal{J} \begin{bmatrix} \psi_{\alpha',0} \\ \psi_{\alpha',1} \\ \psi_{\alpha',2} \end{bmatrix} \tag{80}$$

The overlap matrix computed for the coordinates $\tilde{\psi}_{\alpha',i}$ is then multiplied on the right by a direct sum of three 3×3 matrices $\mathcal{J}$, $I_3 \otimes \mathcal{J}$, and by the transpose of this matrix on the left. This is the overlap matrix for the original unknown coordinates $\psi_{\alpha,i}$.

These $81 = 9^2$ matrix elements must then be tucked into right spots of the $3N_V \times 3N_V$ overlap matrix.

9.2 Potential Energy Matrix:

This is computed by expressing the potential over the element $19 \simeq (3,9,5)$ in terms of its values, and the values of its first derivatives, following the prescription for imposing "boundary conditions" (c.f.,

Eqs.(38-40)). This expression, as well as a similar expression for the wavefunction (c.f., Eq.(40)), is plugged into an expression of the form Eq.(21) and the integrals over the variables ξ, η carried out. These integrals need be done only once. The result is once again a quadratic form in the unknown coefficients $\tilde{\psi}_{3,i}, \tilde{\psi}_{9,i}, \tilde{\psi}_{5,i}$. The matrix elements in the resulting 9×9 matrix are linear functions of the 9 pieces of information derived from the potential: its value at the three vertices and the values of its two first derivatives at these vertices: $\tilde{V}_{\alpha,i}$. The result will have the look of Eq.(24), but the matrix will be much larger and the matrix elements more complicated.

The coefficients $\tilde{V}_{\alpha,i}$ within each matrix element must be transformed back to the known coordinates $V_{\alpha,i}$ by means of a transformation of the type in Eq.(41). The resulting potential energy matrix, in the amplitudes $\tilde{\psi}_{\alpha,i}$, must be transformed back to the matrix describing the quadratic form in the amplitudes $\psi_{\alpha,i}$, as is done for the overlap matrix. This involves multiplying the matrix on the right by $I_3 \otimes \mathcal{J}$ and on the left by its transpose.

These $81 = 9^2$ matrix elements must then be tucked into right spots of the $3N_V \times 3N_V$ potential energy matrix.

9.3 Kinetic Energy Matrix:

The first step is the computation of the gradient of the wavefunction. We use Eq.(16) in the form $\nabla_x \psi = J^{-1} \nabla_\xi \phi$ to make this computation more transparent. Specifically, we write $\partial_\sigma = (J^{-1})_{\sigma,\mu} \partial_\mu$ to abbreviate this relation, where $1 \leq \sigma, \rho \leq 2$ are indices on the real space coordinates $x_\sigma = (x_1, x_2) = (x, y)$ and $1 \leq \mu, \nu \leq 2$ are indices on the canonical coordinates $\xi_\mu = (\xi_1, \xi_2) = (\xi, \eta)$. With this shorthand ($\phi_{\beta,j,\nu} = \partial \phi_{\beta,j} / \partial \xi_\mu$)

$$\partial_\sigma \psi \to (J^{-1})_{\sigma,\mu} \phi_{\alpha,i,\mu} \tilde{\psi}_{\alpha',i} \qquad \nabla\psi \cdot \nabla\psi \to \sum_\sigma \tilde{\psi}_{\beta',j} (J^{-1})_{\sigma,\nu} \phi_{\beta,j,\nu} (J^{-1})_{\sigma,\mu} \phi_{\alpha,i,\mu} \tilde{\psi}_{\alpha',i} \tag{81}$$

The sum over σ is simply a matrix multiplication, leading to the symmetric matrix $((JJ^t)^{-1})_{\nu,\mu}$. The integrals over the product of derivatives of the basis functions can be represented by something with lots of indices. It is useful to represent this as a 2×2 matrix for the four triples $(\beta, j; \alpha, i)$:

$$\mathbf{M}(\beta, j; \alpha, i)_{\nu,\mu} = \int \int \phi_{\beta,j,\nu} \phi_{\alpha,i,\mu} \; d\xi \wedge d\eta \tag{82}$$

The quadratic form representing the kinetic energy is

$$\frac{\hbar^2}{2m} \;\; \tilde{\psi}_{\beta',j} \; \mathrm{Tr} \; \left(\mathbf{M}(\beta, j; \alpha, i) (JJ^t)^{-1} \right) \tilde{\psi}_{\alpha',i} \tag{83}$$

The trace is over 2×2 matrices. In order to construct the quadratic form in the original set of unknown coordinates $\psi_{\alpha',i}$ this 9×9 matrix must be multiplied on the right by $I_3 \otimes \mathcal{J}$ and on the left by its transpose, as usual.

Remind myself to study the symmetry of the integrals in Eq.(43) ASAP.

These $81 = 9^2$ matrix elements must then be tucked into right spots of the $3N_V \times 3N_V$ kinetic energy matrix.

The details are implemented exactly as in Sect. 3.5. There results an equation of the form of Eq.(3.9). The only difference now is that the index i for vertices in Eq.(3.9) is replaced by a double index i, r, where the first index labels the individual vertices $1 \leq i, j \leq N_V$ and the second index $0 \leq r, s \leq 2$ labels the conditions, continuity of the wavefunction, continuity of the two first derivatives, at that vertex. Once again, the equation

$$\langle i, r | (KE + PE - E) | j, s \rangle \langle j, s | \psi \rangle = 0 \tag{84}$$

Table 3: Cubic basis functions for a right tetrahedron with vertices at (0,0,0) and the triples (1,0,0), (0,1,0), and (0,0,1).

$(0,0,0)$	$(1,0,0)$	$(0,1,0)$	$(0,0,1)$
$\phi_1 = 1 - \phi_5 - \phi_9 - \phi_{13}$	$\phi_5 = 3\xi^2 - 2\xi^3$	$\phi_9 = 3\eta^2 - 2\eta^3$	$\phi_{13} = 3\zeta^2 - 2\zeta^3$
$\phi_2 = \xi - 2\xi^2 + \xi^3 - \xi(\eta^2 + \zeta^2)$	$\phi_6 = -\xi^2 + \xi^3$	$\phi_{10} = \eta^2\xi$	$\phi_{14} = \zeta^2\xi$
$\phi_2 = \eta - 2\eta^2 + \eta^3 - \eta(\zeta^2 + \xi^2)$	$\phi_7 = \xi^2\eta$	$\phi_{11} = -\eta^2 + \eta^3$	$\phi_{15} = \zeta^2\eta$
$\phi_4 = \zeta - 2\zeta^2 + \zeta^3 - \zeta(\xi^2 + \eta^2)$	$\phi_8 = \xi^2\zeta$	$\phi_{12} = \eta^2\zeta$	$\phi_{16} = -\zeta^2 + \zeta^3$

(85)

is to be diagonalized and the eigenvectors given the usual tests for convergence to something meaningful.

10 3D: Cubic Functions

10.1 Basis functions

The cubic basis functions for four nodes with four degrees of freedom are:

The remaining four functions $\phi_{17} - \phi_{20}$ fall into two groups: $\phi_* = -\frac{1}{3}x_i x_j + \frac{2}{3}(x_i^2 x_j + x_j^2 x_i)$ $(1 \le i \ne j \le 3)$ and $\phi_{20} = \xi\eta\zeta$.

Remark: There are lots of symmetries among these functions and their derivatives. This means that the number of independent integrals in the overlap, potential, and kinetic matrices is correspondingly reduced.

11 Summary

In finite-**** methods the wavefunction is approximated by its (unknown) values at a whole bunch (N_V) of closely spaced vertices. The approximation is specified by a set of functions, *linearly* scaled by the values of the wavefunctions at the vertices. When these representations for the wavefunction are substituted into the action integral, then the appropriate actions can be carried out on the basis set of functions, and then the integrals can be carried out. The result is a *bilinear* expression in terms of the unknown values at each vertex and their complex conjugates. This expression can be rewritten in matrix form. In this form the matrix that represents the Action Integral is an $N_V \times N_V$ hermitian matrix. When the physics allows the wave function to be real (e.g., bound states), the unknown components are real, the Action Integral is represented by a quadratic form in this unknown values of the wave function, and we have a real symmetric $N_V \times N_V$ matrix to diagonalize. It's eigenvalues approximate the bound states and its eigenvectors determine the values of the different eigenmodes at the various vertices.

12 Appendix A: Wavefunctions on Surfaces

Two-dimensional regions on which we compute wavefunctions need not be flat. The simplest two-dimensional surface on which to compute solutions of the Schrödinger equation is the sphere S^2: the surface $x^2 + y^2 + z^2 = 1$ in R^3. The solutions are already known: they are the spherical harmonics $Y_m^l(\theta, \phi)$.

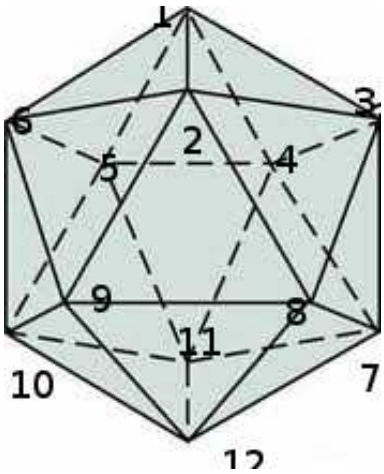

Figure 4: The icosahedron is one of the five Platonic solids, and one of only two whose faces are all triangles. This figure presents a crude approximation to the sphere. The vertices are numbered as shown in this figure.

We can attempt to compute these functions using the Finite Element Method to illustrate how this works for nonflat spaces. We choose a very simple case — the icosahedron, one of the Platonic solids. Ee do this because there is only one computation to do.

An icosahedron is shown in Fig. 4. There are 12 vertices, 30 edges, and 20 faces. We number the vertices as indicated. In this numbering scheme the sum of two vertices at opposite ends of a diameter is the lucky number 13. Each vertex is joined to five other vertices and contained in five triangles. Each triangle is equilateral. The connectivity is:

1	2	3	4	5	6
2	1	3	6	8	9
3	1	2	4	7	8
4	1	3	5	7	11
5	1	4	6	10	11
6	1	2	5	9	10
7	12	11	8	4	3
8	12	9	7	3	2
9	12	10	8	6	2
10	12	11	9	6	5
11	12	10	7	5	4
12	11	10	9	8	7

(86)

The kinetic energy is computed from Eq. (23). Each triangle makes the same contribution to the kinetic energy. If we choose spacial coordinates x, y for one of the triangles so that the vertices are at $(0,0), (1,0), (\frac{1}{2}, \frac{\sqrt{3}}{2})$, the relation between the global and local coordinates is

$$\left[\begin{array}{cc} x & y \end{array}\right] = \left[\begin{array}{cc} \xi & \eta \end{array}\right] \left[\begin{array}{cc} 1 & 0 \\ \frac{1}{2} & \frac{\sqrt{3}}{2} \end{array}\right] = \left[\begin{array}{cc} \xi & \eta \end{array}\right] J \tag{87}$$

From this we compute

$$(J^{-1})^t(J^{-1}) = (JJ^t)^{-1} = \begin{bmatrix} \frac{4}{3} & -\frac{2}{3} \\ -\frac{2}{3} & \frac{4}{3} \end{bmatrix} \tag{88}$$

Using this result in Eq.(24) we find for the contribution to the Kinetic Energy matrix

$$\frac{2}{3}\begin{bmatrix} 2 & -1 & -1 \\ -1 & 2 & -1 \\ -1 & -1 & 2 \end{bmatrix} \tag{89}$$

Construction of the 12×12 kinetic energy matrix is now a piece of cake. It is

$$2 \times \frac{2}{3}\begin{bmatrix} 5 & -1 & -1 & -1 & -1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 5 & -1 & 0 & 0 & -1 & 0 & -1 & -1 & 0 & 0 & 0 \\ -1 & -1 & 5 & -1 & 0 & 0 & -1 & -1 & 0 & 0 & 0 & 0 \\ -1 & 0 & -1 & 5 & -1 & 0 & -1 & 0 & 0 & 0 & -1 & 0 \\ -1 & 0 & 0 & -1 & 5 & -1 & 0 & 0 & 0 & -1 & -1 & 0 \\ -1 & -1 & 0 & 0 & -1 & 5 & 0 & 0 & -1 & -1 & 0 & 0 \\ 0 & 0 & -1 & -1 & 0 & 0 & 5 & -1 & 0 & 0 & -1 & -1 \\ 0 & -1 & -1 & 0 & 0 & 0 & -1 & 5 & -1 & 0 & 0 & -1 \\ 0 & -1 & 0 & 0 & 0 & -1 & 0 & -1 & 5 & -1 & 0 & -1 \\ 0 & 0 & 0 & 0 & -1 & -1 & 0 & 0 & -1 & 5 & -1 & -1 \\ 0 & 0 & 0 & -1 & -1 & 0 & -1 & 0 & 0 & -1 & 5 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & -1 & -1 & -1 & -1 & 5 \end{bmatrix} \tag{90}$$

For example, the sixth row is obtained as follows. The vertex 6 is contained in five triangles, so place $5 \times 2 \times \frac{2}{3}$ in the $(6,6)$ position in this matrix. The vertices connected to vertex 6 in triangles are $(1,2,5,9,10)$ (each of these vertices is in 2 triangles), so place $1 \times 2 \times \frac{-2}{3}$ in these columns in the row 6 of this matrix. The common factor $\frac{4}{3}$ has been factored out of this matrix. All rows are computed similarly.

This real symmetric matrix has eigenvalues $0, 5 \pm \sqrt{5}, 6$. The eigenvalue 0 is immediate: the sum of the elements in each row is zero, so one eigenvector is the Goldstone mode (all components of the eigenvector are equal). This eigenvalue is nondegenerate and corresponds to the $l = 0$ S state. The eigenvalue $5 - \sqrt{5}$ is triply degenerate, and corresponds to the $l = 1$ P state. The eigenvalue 6 is 5-fold degenerate and corresponds to the $l = 2$ D state. There are three $(12 - 1 - 3 - 5)$ remain eigenvalues, all are $5 + \sqrt{5}$ that don't coorrespond to any angular momentum states, since we have truncated the discretization to too small (12) a number of vertices.

$$\begin{array}{cccccccccccc} 0 & & 5-\sqrt{5} & & & & 6 & & & & 5+\sqrt{5} & \\ \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} & ; & \begin{bmatrix} -1 \\ 0 \\ 0 \\ -r \\ -1 \\ -r \\ r \\ 1 \\ r \\ 0 \\ 0 \\ 0 \end{bmatrix} \begin{bmatrix} 0 \\ -1 \\ 0 \\ 1 \\ r \\ -r \\ r \\ -r \\ -1 \\ 0 \\ 1 \\ 0 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ -1 \\ -r \\ r \\ 1 \\ -1 \\ -r \\ r \\ 1 \\ 0 \\ 0 \end{bmatrix} & ; & \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ -1 \\ -1 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ -1 \\ -1 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ -1 \\ -1 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ -1 \\ -1 \\ 0 \\ 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ -1 \\ -1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} & ; & \begin{bmatrix} -1 \\ 0 \\ 0 \\ s \\ -1 \\ s \\ -s \\ 1 \\ -s \\ -s \\ 0 \\ 1 \end{bmatrix} \begin{bmatrix} 0 \\ -1 \\ 0 \\ 1 \\ -s \\ s \\ -s \\ s \\ -1 \\ 0 \\ 1 \\ 0 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ -1 \\ s \\ -s \\ 1 \\ -1 \\ s \\ -s \\ 1 \\ 0 \\ 0 \end{bmatrix} \end{array} \tag{91}$$

All the components of the eigenvector with $E = 0$ are equal. This is the S state wavefunction. In this representation it looks like a Goldstone mode.

The next triplet of eigenvectors is energy-degenerate, with $E = 5 - \sqrt{5}$. In these eigenvectors $r = (\sqrt{5} - 1)/2$. Each of these three eigenfunctions has one nodal line.

The next quintet eigenvectors is energy-degenerate, with $E = 6$. Each of these five wavefunctions has two nodal lines.

The last three eigenvectors do not corresponding to any rotational invariance. They are present because this problem has "12" degrees of freedom: that is, there are 12 vertices. There must be 12 eigenvectors, and symmetry accounts for $1+3+5 = 9$ of them. For these eigenvectors $s = (\sqrt{5}+1)/2$ and the nodal line structure is evident in the plots of these eigenfunctions.

We notice that the numerical results are different from the analytic results. Numerically, the energy ratio between the quintet and triplet states is $6/(5 - \sqrt{5}) = 2.1708$ whereas analytically this ratio is $(2 \times 3)/(1 \times 2) = 3$. This ratio can't be tampered with by adjusting the values of the matrix elements, by symmetry. If the sums of the elements in each row/column did not vanish the S state would not have the properties that it displays. We expect these ratios to approach their analytic values $((L + 2)/L)$ as the number of vertices in a tesselation of a sphere into triangles grows.