Quantum Mechanics on Curves & Surfaces

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Abstract

In order to describe the quantum mechanics of a particle confined to a curve or a surface in R^3 Schrödinger's equation must be modified in two ways. The kinetic energy operator must be written in terms of the metric g^{ij} induced on the surface from the flat space metric $G_{ij} = \delta_{ij}$. The potential energy term must be modified by the inclusion of a geometric potential, necessary to constrain the particle to the curve or surface.

1 Preliminaries

Schrödinger's Action Integral on a manifold $\mathcal{M}$ embedded in R^3 has the form

$$I = \int \left[\frac{\hbar^2}{2m} g^{ij} \partial_i \psi \partial_j \psi + V(\mathbf{x}) \psi^2 \right] dS = 0 \tag{1}$$

This integral over the manifold is minimized (made stationary) subject to the condition that the solution ψ is nonzero. This condition is usually imposed through use of a Lagrange multiplier.

1.1 Geometric Parts of the Action Integral

The metric tensor g^{ij} measures distances in the manifold. It is induced from the Euclidean metric on R^3. The metric tensor on the manifold is determined by equating distances as measured in the manifold with distances in R^3. For example, if du^i are the coordinate differences between two points in $\mathcal{M}$ and dx^α are the distances between these points in a Euclidean coordinate system in R^3,

$$\delta_{\alpha\beta} dx^\alpha dx^\beta = ds^2 = g_{ij} du^i du^j \tag{2}$$

and the two (covariant) metrics are related to each other by taking the appropriate partial derivatives.

The potential is the sum of two terms: $V(\mathbf{x}) = V_{\rm physical}(\mathbf{x}) + V_{\rm geometric}(\mathbf{x})$. The physical potential describes purely physical (electric, magnetic) interactions. The geometric or confining potential is present in order to confine the particle to the D-dimensional manifold $\mathcal{M}$ in R^3. It is expressed in terms of the principal curvatures R_i at each point

$$V_{\rm geom} = \frac{\hbar^2}{2m}\left(-\frac{1}{2}\sum_{i=1}^{D}\frac{1}{R_i^2} + \left(\frac{1}{2}\sum_{i=1}^{D}\frac{1}{R_i}\right)^2\right) \tag{3}$$

We will be principally interested in cases in which the physical potential is absent.

We consider two distinct cases. The first case is that of closed curves (knots) in R^3. The second case is of two-dimensional surfaces in R^3.

2 Curves

2.1 Parameterization

A closed curve is usefully parameterized by trigonometric functions $\cos(\theta+\phi)$. There is a theorem that every knot is a "Chebyschev" knot: $\mathcal{K} = C(a,b,c,\phi)$, where a, b, c are relatively prime integers and $C(a,b,c,\phi)$ describes the (x,y,z) components as $(x,y,z) = (T_a(\cos(\theta)), T_b(\cos(\theta)), T_c(\cos(\theta)+\phi)) = (\cos(a\theta),$ $\cos(b\theta), \cos(c\theta+\phi))$ For now we simply use the parameterization $(x(\theta), y(\theta), z(\theta))$.

2.2 Metric

We need a metric tensor to describe the kinetic part of the Schrödinger action. It is determined from

$$ds^2 = g_{ij}dx^i dx^j = g_{\theta\theta}d\theta^2 \Rightarrow g_{\theta\theta} = \frac{d\mathbf{x}}{d\theta}\cdot\frac{d\mathbf{x}}{d\theta} \tag{4}$$

Here $\frac{d\mathbf{x}}{d\theta}$ is proportional to the tangent vector $\hat{\mathbf{t}}$, in fact $\hat{\mathbf{t}} = \frac{d\mathbf{x}}{d\theta}/|\frac{d\mathbf{x}}{d\theta}|$. The kinetic energy term in the Schrödinger action is

$$\frac{\hbar^2}{2m}g^{\theta\theta}\left(\frac{d\psi}{d\theta}\right)^2 = \frac{\hbar^2}{2m}\left(\frac{d\mathbf{x}}{d\theta}\cdot\frac{d\mathbf{x}}{d\theta}\right)^{-1}\left(\frac{d\psi}{d\theta}\right)^2 \tag{5}$$

2.3 Geometric Potential

The geometric potential needed to confine a particle to the curve is $\frac{\hbar^2}{2m}\left(-\frac{1}{4R^2}\right)$. Here R is the radius of curvature at a point, related to the curvature κ at a point by $R(\theta)\kappa(\theta) = 1$. The curvature is related to the derivative of the unit tangent vector $\hat{\mathbf{t}}$ by

$$\frac{d\hat{\mathbf{t}}}{d\theta} = \kappa\hat{\mathbf{n}} \Rightarrow \kappa^2 = \frac{d\hat{\mathbf{t}}}{d\theta}\cdot\frac{d\hat{\mathbf{t}}}{d\theta} \tag{6}$$

Here $\hat{\mathbf{n}}$ is the unit normal to the curve and $\hat{\mathbf{t}}\cdot\hat{\mathbf{n}} = 0$. Then

$$\kappa\hat{\mathbf{n}} = \frac{d\hat{\mathbf{t}}}{d\theta} = \frac{d}{d\theta}\frac{\dot{\mathbf{x}}}{\sqrt{\dot{\mathbf{x}}\cdot\dot{\mathbf{x}}}} = \frac{\ddot{\mathbf{x}}}{\sqrt{\dot{\mathbf{x}}\cdot\dot{\mathbf{x}}}} - \frac{\dot{\mathbf{x}}(\dot{\mathbf{x}}\cdot\ddot{\mathbf{x}})}{(\dot{\mathbf{x}}\cdot\dot{\mathbf{x}})^{3/2}} = \frac{\ddot{\mathbf{x}}(\dot{\mathbf{x}}\cdot\dot{\mathbf{x}}) - \dot{\mathbf{x}}(\dot{\mathbf{x}}\cdot\ddot{\mathbf{x}})}{(\dot{\mathbf{x}}\cdot\dot{\mathbf{x}})^{3/2}} \tag{7}$$

and

$$\kappa^2 = \frac{1}{R^2} = \frac{(\dot{\mathbf{x}}\cdot\dot{\mathbf{x}})(\ddot{\mathbf{x}}\cdot\ddot{\mathbf{x}}) - (\dot{\mathbf{x}}\cdot\ddot{\mathbf{x}})(\dot{\mathbf{x}}\cdot\ddot{\mathbf{x}})}{\sqrt{\dot{\mathbf{x}}\cdot\dot{\mathbf{x}}}} \tag{8}$$

Here $\dot{\mathbf{x}} = d\mathbf{x}/d\theta$, etc.

2.4 Schrödinger Action and Equation

The Schrodinger Action Integral is

$$\mathcal{I} = \frac{\hbar^2}{2m}\oint\left(\frac{1}{\dot{\mathbf{x}}\cdot\dot{\mathbf{x}}}\frac{d\psi^*}{d\theta}\frac{d\psi}{d\theta} - \frac{1}{4}\frac{(\dot{\mathbf{x}}\cdot\dot{\mathbf{x}})(\ddot{\mathbf{x}}\cdot\ddot{\mathbf{x}}) - (\dot{\mathbf{x}}\cdot\ddot{\mathbf{x}})(\dot{\mathbf{x}}\cdot\ddot{\mathbf{x}})}{\sqrt{\dot{\mathbf{x}}\cdot\dot{\mathbf{x}}}}\psi^*\psi\right)\,d\theta \tag{9}$$

We search for solutions that make $\mathcal{I}$ stationary, subject to the normalization condition $\oint\psi^*\psi d\theta = 1$.

The arguments within the action integral are all functions of the angle θ that the parameterization of the knot depends on. For Chebyshev knots (a,b,c) with $\phi = 0, \pm\pi/2, \pi$ the following symmetries hold

$$\begin{array}{ccc} & \theta\to-\theta & \\ \dot{x}\cdot\dot{x} & \to & +\dot{x}\cdot\dot{x} \\ \dot{x}\cdot\ddot{x} & \to & -\dot{x}\cdot\ddot{x} \\ \ddot{x}\cdot\ddot{x} & \to & +\ddot{x}\cdot\ddot{x} \end{array} \tag{10}$$

As a result the argument of the action integral has a two-fold symmetry and the set of solutions breaks into two subsets: one with even symmetry under $\theta\to-\theta$ and the other with odd symmetry. The even and odd sets can be expressed as sines and cosines:

$$\psi_{\rm even}(\theta) = \frac{a_0}{2}\cos(0\theta) + \sum_{j>0} a_j\cos(j\theta) \qquad \psi_{\rm odd}(\theta) = \sum_{j>0} b_j\sin(j\theta) \tag{11}$$

The variational equation for the amplitudes a_j is

$$\mathcal{I}\to\sum_{j'j\geq 0} a_{j'}\left(\mathcal{KE}_{j'j} + \mathcal{V}_{j'j}\right)a_j \tag{12}$$

and the matrix eigenvalue equation is

$$\sum_{j\geq 0}\left(\mathcal{KE}_{j'j} + \mathcal{V}_{j'j}a_j - \frac{\pi E}{\hbar^2/2m}\delta_{j'j}\right) = 0 \tag{13}$$

The matrix elements are

$$\begin{array}{rcl} \mathcal{KE}_{j'j} & = & \oint d\theta\ j'\sin(j'\theta)g^{\theta\theta}(a,b,c)j\sin(j\theta) \\ \mathcal{V}_{j'j} & = & \oint d\theta\ \cos(j'\theta)\left(-\frac{1}{4}\kappa^2(a,b,c)\right)\cos(j\theta) \end{array} \tag{14}$$

The functions $g^{\theta\theta}(a,b,c)$ and $\kappa^2(a,b,c)$ are well-defined by Eqs. (4) and (8) once the knot has been chosen and its Chebyshev expression is introduced to parameterize the knot.

The variational expression for odd functions is similar, with the obvious replacements.

Schrödinger's second order differential equation is obtained in the usual fashion by integrating by parts:

$$-\frac{d}{d\theta}g^{\theta\theta}(a,b,c)\frac{d\psi}{d\theta} - \frac{1}{4}\kappa^2(a,b,c)\psi - \frac{E}{\hbar^2/2m}\psi = 0 \tag{15}$$

2.5 Propagation Along a Curve

Propagation along the curve is governed by Eq. (15). Since this is an ordinary differential equation it is useful to write this as a pair of couple ordinary differential equations. We do this by defining $A(\theta) = \psi(\theta)$ and $B(\theta) = g^{\theta\theta}dA(\theta)/d\theta$. The equations of motion are, in matrix form

$$\frac{d}{d\theta}\begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} 0 & 1/g^{\theta\theta} \\ -(E-V) & 0 \end{bmatrix}\begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} 0 & g_{\theta\theta} \\ -(E-V) & 0 \end{bmatrix}\begin{bmatrix} A \\ B \end{bmatrix} \tag{16}$$

This equation must hold for an arbitrary initial condition, so it holds for a 2×2 transfer matrix M:

$$\frac{d}{d\theta}\begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix} = \begin{bmatrix} 0 & g_{\theta\theta} \\ -(E-V) & 0 \end{bmatrix}\begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix} \tag{17}$$

This equation can be integrated from an initial value θ_i to some final value θ_f with $M(\theta_i,\theta_i) = I_2$. The matrix $M(\theta_f,\theta_i)$ relates the amplitudes at the initial position θ_i with those at the final position θ_f.

2.6 Transfer and Scattering Matrix

At any point along the curve the wave function can be written in terms of the coefficients $A = \psi$ and $B = g^{**}\psi'$ or in terms of waves travelling to the right ($W_+e^{+ik\theta}$) and to the left ($W_-e^{-ik\theta}$). Equating the wavefunction and its derivative in these two representations leads to the relation

$$\begin{bmatrix} \psi = A \\ \psi' = g_{**}B \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ ik & -ik \end{bmatrix}\begin{bmatrix} e^{+ik\theta} & 0 \\ 0 & e^{-ik\theta} \end{bmatrix}\begin{bmatrix} W_+ \\ W_- \end{bmatrix} \tag{18}$$

The two amplitudes W_+, W_- are

$$\begin{bmatrix} W_+ \\ W_- \end{bmatrix} = \begin{bmatrix} e^{+ik\theta} & 0 \\ 0 & e^{-ik\theta} \end{bmatrix}^{-1}\begin{bmatrix} 1 & 1 \\ ik & -ik \end{bmatrix}^{-1}\begin{bmatrix} 1 & 0 \\ 0 & g^{**} \end{bmatrix}^{-1}\begin{bmatrix} A \\ B \end{bmatrix} \tag{19}$$

This result can be combined with the expression for the relation between the amplitudes at θ_i and θ_f

$$\begin{bmatrix} A \\ B \end{bmatrix}_f = M(\theta_f, \theta_i) \begin{bmatrix} A \\ B \end{bmatrix}_i \tag{20}$$

to give an expression for the transfer matrix for the amplitudes between these points:

$$\begin{bmatrix} W_+ \\ W_- \end{bmatrix}_f = (GK\Theta)_f^{-1} M(\theta_f, \theta_i)(GK\Theta)_i \begin{bmatrix} W_+ \\ W_- \end{bmatrix}_i \tag{21}$$

where $G = \begin{bmatrix} 1 & 0 \\ 0 & g^{**} \end{bmatrix}$, $K = \begin{bmatrix} 1 & 1 \\ ik & -ik \end{bmatrix}$, and $\Theta = \begin{bmatrix} e^{+ik\theta} & 0 \\ 0 & e^{-ik\theta} \end{bmatrix}$.

The scattering matrix S relates the incoming amplitudes $W_{+,i}, W_{-,f}$ to the outgoing amplitudes $W_{+,f}, W_{-,i}$:

$$\begin{bmatrix} W_{+,f} \\ W_{-,i} \end{bmatrix} = S \begin{bmatrix} W_{+,i} \\ W_{-,f} \end{bmatrix} \tag{22}$$

The matrix elements of the S matrix are obtained from those of the transfer matrix T in Eq. (21) by simple algebraic manipulations.

3 Surfaces

Although it is often possible to construct analytic representations of surfaces in R^3, we will often represent them by specifying a set of *vertices* $\mathbf{x}_i$ ($i = 1, 2, \cdots N_V$) that are distributed over the surface. This representation is called a tessellation. We describe how to construct the geometric inputs to the Schrödinger Action Integral for both the analytic rerpesentation and the tessellation of the surface.

3.1 Gauss Fundamental Forms

Gauss introduced two fundamental forms in order to describe the properties of surfaces embedded in R^3:

I	Distance	ds^2	=	$Edx^2 + 2Fdxdy + Gdy^2$
II	Curvature	$2dz$	=	$Ldx^2 + 2Mdxdy + Ndy^2$

Here ds is the distance between the origin and a point with coordinates (dx, dy) in the surface and $2dz$ is twice the distance between a point with coordinates (dx, dy) in the surface and with the same coordinates in the plane tangent to the surface at the origin. In order to construct the Schrödinger action integral we will have to construct: the first fundamental form for the surface at a point in order to construct the kinetic energy part of the integral; the second fundamental form for the surface at the same point in order to construct the geometric potential energy part of the integral.

3.2 Construction of the Metric

Choose a vertex $\mathbf{x_0}$ and a sufficient number ($n \geq 3$) of neighbors of this point. Set $\mathbf{\Delta x}_i = \mathbf{x}_i - \mathbf{x}_0$ and treat it as a three-component row vector. Nearby points lie approximately in a plane. The plane can be determined by carrying out a singular value decomposition on the 3×3 covariance matrix constructed from coordinate differences:

$$CM = \sum_{i=1}^{n} \mathbf{\Delta x}_i^t \mathbf{\Delta x}_i = \sum_{i=1}^{n} (\mathbf{x}_i - \mathbf{x}_0)^t (\mathbf{x}_i - \mathbf{x}_0) \tag{23}$$

The two large eigenvalues $\lambda_1 \geq \lambda_2 \gg \lambda_3 \geq 0$ are associated with eigenvectors $\mathbf{e}_1$ and $\mathbf{e}_2$ that span the plane tangent to the surface at $\mathbf{x}_0$. The third eigendirection $\mathbf{e}_3$ is perpendicular to the surface at $\mathbf{x}_0$: it is in the direction of the gradient to the surface at $\mathbf{x}_0$. The three unit vectors $\mathbf{e}_i$ are orthonormal.

In the tangent plane Gauss' First Fundamental Form is $g_{ij} = \mathbf{e}_i \cdot \mathbf{e}_j$ so the kinetic energy term $g^{ij}\partial_i\psi\partial_j\psi$ is the straightforward Euclidean operator. The kinetic energy term is created without the complication of computing the matrix elements $(E, F, G) = (1, 0, 1)$. To construct the kinetic energy matrix for the triangle with three vertices $\mathbf{x}_0, \mathbf{x}_i, \mathbf{x}_j$ it is sufficient to project the differences $(\mathbf{x}_i - \mathbf{x}_0)$ onto the plane: $\Delta x_i = (\mathbf{x}_i - \mathbf{x}_0) \cdot \mathbf{e}_1$, $\Delta y_i = (\mathbf{x}_i - \mathbf{x}_0) \cdot \mathbf{e}_2$, and similarly for $\mathbf{x}_j$, and then use the results for the kinetic energy operator on a triangle in a plane.

3.3 Construction of the Geometric Potential

The geometric potential at a point on a curved surface is a function of the principal radii of curvature at that point:

$$V_{\text{geometric}}(\mathbf{x}) = -\frac{\hbar^2}{2m}\frac{1}{4}\left(\frac{1}{R_1} - \frac{1}{R_2}\right)^2 \tag{24}$$

Here R_1, R_2 are the principal radii of curvature of the surface at $\mathbf{x}_0$. These in turn are the reciprocals of the eigenvalues of the 2×2 matrix $\begin{bmatrix} L & M \\ M & N \end{bmatrix}$ of Gauss' Second Fundamental Form when the First Fundamental Form is the identity matrix I_2.

These cofficients are determined as follows. Construct the matrices

$$\begin{bmatrix} dx_1 dx_1 & 2dx_1 dy_1 & dy_1 dy_1 \\ dx_2 dx_2 & 2dx_2 dy_2 & dy_2 dy_2 \\ \vdots & \vdots & \vdots \\ dx_n dx_n & 2dx_n dy_n & dy_n dy_n \end{bmatrix} \begin{bmatrix} L \\ M \\ N \end{bmatrix} = \begin{bmatrix} 2dz_1 \\ 2dz_2 \\ \vdots \\ 2dz_n \end{bmatrix} \text{ or } T \begin{bmatrix} L \\ M \\ N \end{bmatrix} = \begin{bmatrix} 2dz \end{bmatrix} \tag{25}$$

In this expression $(dx_i, dy_i, dz_i) = (\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3) \cdot (\mathbf{x}_i - \mathbf{x}_0)$. Multiply both sides by the transpose matrix T^t. The matrix $T^t T$ is nonsingular. Multiply both sides by its inverse to obtain

$$\begin{bmatrix} L \\ M \\ N \end{bmatrix} = (T^t T)^{-1} T^t \begin{bmatrix} 2dz \end{bmatrix} \tag{26}$$

Now construct the eigenvalues $\lambda_1 = 1/R_1, \lambda_2 = 1/R_2$ of $\begin{bmatrix} L & M \\ M & N \end{bmatrix}$ and use these values in Eq. (24) for the geometric potential.

3.4 Parameterization Patches

There are many ways to parameterize a surface. One useful method involves mapping a planar patch with coordinates (u, v) into R^3 by means of $(u, v) \to \mathbf{x} \in R^3$ with $\mathbf{x}(\mathbf{u}) = (x(u, v), y(u, v), z(u, v))$. Then tangent vectors to the surface at a point $\mathbf{x}_0$ are

$$\mathbf{t}_u = \frac{\partial \mathbf{x}}{\partial u} = \mathbf{x}_u \qquad \mathbf{t}_v = \frac{\partial \mathbf{x}}{\partial v} = \mathbf{x}_v \qquad \mathbf{N} = \mathbf{t}_u \times \mathbf{t}_v \tag{27}$$

These vectors are not normalized. The unit normal vector is $\hat{\mathbf{N}} = \mathbf{x}_u \times \mathbf{x}_v / |\mathbf{x}_u \times \mathbf{x}_v|$. In this parameterization the First and Second Fundamental forms are

$$I = \begin{bmatrix} E & F \\ F & G \end{bmatrix} = \begin{bmatrix} \mathbf{x}_u \cdot \mathbf{x}_u & \mathbf{x}_u \cdot \mathbf{x}_v \\ \mathbf{x}_v \cdot \mathbf{x}_u & \mathbf{x}_v \cdot \mathbf{x}_v \end{bmatrix} \qquad II = \begin{bmatrix} L & M \\ M & N \end{bmatrix} = \begin{bmatrix} \mathbf{x}_{uu} \cdot \hat{\mathbf{N}} & \mathbf{x}_{uv} \cdot \hat{\mathbf{N}} \\ \mathbf{x}_{vu} \cdot \hat{\mathbf{N}} & \mathbf{x}_{vv} \cdot \hat{\mathbf{N}} \end{bmatrix} \tag{28}$$

The principal curvatures $\kappa_1 = 1/R_1, \kappa_2 = 1/R_2$ are obtained by solving the eigenvalue equation:

$$([II] - \kappa [I]) \begin{pmatrix} du \\ dv \end{pmatrix} = 0 \tag{29}$$

The corresponding eigenvectors are the principal directions.

If only the principla curvatures are required, then it is useful to observe that the eigenvalues can be obtained by rewriting Eq. (28) as

$$K - \kappa I_2 = [II] [I]^{-1} - \kappa I_2 = [I]^{-1} [II] - \kappa I_2 \tag{30}$$

The geometric potential is then

$$V_{\text{geom}} = \frac{\hbar^2}{2m} \left(\left(\frac{1}{2} \text{tr}(K) \right)^2 - \frac{1}{2} \text{tr}(K^2) \right) \tag{31}$$

This eliminates the need for diagonalizing a matrix. If $[II] [I]^{-1} = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$ then $(\kappa_1 - \kappa_2)^2 = (1/R_1 - 1/r_2)^2 = (a + d)^2 - 4(ad - bc)$.

The kinetic energy can also be determined in this parameterization. Assume we have three vertices in the parameterizing patch: $\mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_3$ with coordinates $(u, v)_i$, $i = 1, 2, 3$. Then the basis function at vertex 1 is

$$\phi_1(u,v) = \left| \begin{array}{ccc} u & v & 1 \\ u_2 & v_2 & 1 \\ u_3 & v_3 & 1 \end{array} \right| / \left| \begin{array}{ccc} u_1 & v_1 & 1 \\ u_2 & v_2 & 1 \\ u_3 & v_3 & 1 \end{array} \right| \tag{32}$$

with ϕ_2, ϕ_3 defined similarly. The gradient of $\psi(u,v) = c_1\phi_1 + c_2\phi_2 + c_3\phi_3$ is constructed from

$$\frac{\partial \psi^*}{\partial u} = \begin{pmatrix} c_1 & c_2 & c_3 \end{pmatrix} \begin{pmatrix} v_2 - v_3 \\ v_3 - v_1 \\ v_1 - v_2 \end{pmatrix} / D \qquad \frac{\partial \psi^*}{\partial v} = -\begin{pmatrix} c_1 & c_2 & c_3 \end{pmatrix}^* \begin{pmatrix} u_2 - u_3 \\ u_3 - u_1 \\ u_1 - u_2 \end{pmatrix} / D \tag{33}$$

where D is the denominator in Eq. (32). The integral over this simplex is $\int\int g^{\alpha\beta}\psi_\alpha\psi_\beta\sqrt{\det g_{**}}du \wedge dv$. The derivatives ψ_α are independent of (u,v) and the metric tensor can be approximated as the value of the metric at any of the three vertices, or even the average of the values at the three vertices. The intermediate result is

$$\mathcal{K} = \frac{A}{D^2} \begin{pmatrix} c_1 & c_2 & c_3 \end{pmatrix} \begin{pmatrix} v_2 - v_3 & -(u_2 - u_3) \\ v_3 - v_1 & -(u_3 - u_1) \\ v_1 - v_2 & -(u_1 - u_2) \end{pmatrix} \begin{bmatrix} g^{11} & g^{12} \\ g^{21} & g^{22} \end{bmatrix} \times$$

$$\begin{pmatrix} v_2 - v_3 & v_3 - v_1 & v_1 - v_2 \\ -(u_2 - u_3) & -(u_3 - u_1) & -(u_1 - u_2) \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} \times \sqrt{\det g_{**}} \tag{34}$$

Here A is $\frac{1}{2}D$. We have explicit expressions for the other terms in this expression:

$$\sqrt{\det g_{**}} = \sqrt{EG - F^2} \qquad g^{**} = \frac{1}{EG - F^2} \begin{bmatrix} G & -F \\ -F & E \end{bmatrix} \tag{35}$$

Putting this all together, we find

$$\mathcal{K} = \frac{1}{2D} \frac{1}{\sqrt{EG - F^2}} \begin{pmatrix} c_1 & c_2 & c_3 \end{pmatrix} M \begin{bmatrix} E & F \\ F & G \end{bmatrix} M^t \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} \tag{36}$$

with

$$M = \begin{bmatrix} u_2 - u_3 & v_2 - v_3 \\ u_3 - u_1 & v_3 - v_1 \\ u_1 - u_2 & v_1 - v_2 \end{bmatrix} \tag{37}$$

For the flat metric $g^{**} = \delta^{ij}$ the result reduces to the standard result shown in Eq. (40).

3.5 Constraint Functions

Another useful way to describe a surface is through a function $f(x, y, z) =$ const. A single constraint on three variables typically produces a smooth two-dimensional surface. In the event a function is not prescribed, the surface can be locally parameterized in this way by fitting the vertices in the neighborhood of a vertex of interest ($\mathbf{x}_0$) to a smooth function using a best fit or singular value procedure (Appendix). For our purposes a fit containing only the first and second degree terms in the Taylor series expansion is sufficient.

The normal at a point $\mathbf{x}_0$ is $\mathbf{N} = \boldsymbol{\nabla} f|_{\mathbf{x}_0}$. Tangent vectors to the surface are conveniently obtained as follows. Determine the magnitude of the components of $\mathbf{N}$. If $|f_y = f_2|$ is smaller than the other two partial derivatives, then take the first tangent vector as $\mathbf{t}_1 \simeq (f_3, 0, -f_1)$ and the other tangent vector as $\mathbf{t}_2 \simeq \mathbf{N} \times \mathbf{t}_1$.

In the tangent plane when $\mathbf{t}_1$ and $\mathbf{t}_2$ are normalized to one, the metric tensor is flat: $g_{ij} = g^{ij} = \delta_{ij}$ and construction of the kinetic energy matrix elements proceeds as in flat space.

The curvature form is obtained from the first and second derivatives as follows. Construct the 3×3 matrix K as follows:

$$K = \frac{1}{|\mathbf{N}|}\left(f_{ij} - \frac{(f_{ir}f_r)(f_s f_{sj})}{(f_t f_{tu} f_u)}\right) \tag{38}$$

The matrix K has one vanishing eigenvalue, corresponding to the normal direction. The other two eigenvalues are the curvatures in the principal directions. As in subsection (3.4), the geometric potential is

$$V_{\text{geom}} = \frac{\hbar^2}{2m}\left(\left(\frac{1}{2}\text{tr }(K)\right)^2 - \frac{1}{2}\text{tr }(K^2)\right) \tag{39}$$

This again eliminates the need for diagonalizing a matrix.

3.6 Constructing the FEM Matrices

The kinetic energy matrix can be constructed using the vector positions $\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3$ of the three vertices of a triangle. The matrix elements are expressed in terms of inner products as follows

$$\mathcal{K}_{\triangle(\mathbf{x_1x_2x_3})} = \frac{1}{4A}\begin{bmatrix} (\mathbf{x}_2-\mathbf{x}_3)\cdot(\mathbf{x}_2-\mathbf{x}_3) & -(\mathbf{x}_1-\mathbf{x}_3)\cdot(\mathbf{x}_2-\mathbf{x}_3) & -(\mathbf{x}_1-\mathbf{x}_2)\cdot(\mathbf{x}_3-\mathbf{x}_2) \\ -(\mathbf{x}_2-\mathbf{x}_3)\cdot(\mathbf{x}_1-\mathbf{x}_3) & (\mathbf{x}_3-\mathbf{x}_1)\cdot(\mathbf{x}_3-\mathbf{x}_1) & -(\mathbf{x}_2-\mathbf{x}_1)\cdot(\mathbf{x}_3-\mathbf{x}_1) \\ -(\mathbf{x}_3-\mathbf{x}_2)\cdot(\mathbf{x}_1-\mathbf{x}_2) & -(\mathbf{x}_3-\mathbf{x}_1)\cdot(\mathbf{x}_2-\mathbf{x}_1) & (\mathbf{x}_1-\mathbf{x}_2)\cdot(\mathbf{x}_1-\mathbf{x}_2) \end{bmatrix} \tag{40}$$

where A is the area of the triangle, $2A = |(\mathbf{x}_2 - \mathbf{x}_1)\times(\mathbf{x}_3 - \mathbf{x}_1)|$.

The potential energy matrix over the same triangle is

$$\mathcal{V}_{\triangle(\mathbf{x_1x_2x_3})} = \frac{A}{60}\begin{bmatrix} (6,2,2) & (2,2,1) & (2,1,2) \\ (2,2,1) & (2,6,2) & (1,2,2) \\ (2,1,2) & (1,2,2) & (2,2,6) \end{bmatrix} \tag{41}$$

where the meaning of $(2,1,2)$ in the $(1,3)$ matrix element is $(2,1,2) \to 2 \times V(\mathbf{x}_1) + 1 \times V(\mathbf{x}_2) + 2 \times V(\mathbf{x}_3)$.

The overlap matrix is obtained from the potential energy matrix by inserting the constant potential $V = 1$ everywhere:

$$\mathcal{O}_{\triangle(\mathbf{x_1 x_2 x_3})} = \frac{A}{12} \begin{bmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{bmatrix} \tag{42}$$

3.7 Periodic Boundary Conditions

Application of Dirichlet and von Neumann boundary conditions within the Finite Element Method is well-understood. Here is how to impose periodic boundary conditions. Assume the matrix elements have been computed for two vertices, and the vertices are labelled $i = (1,2,3)$ for one and $r = (4,5,6)$ for the second. Suppose also that after all the quadratic forms have been constructed, we impose the condition that vertex 1 is the same as vertex 6. Then $c_1 = c_6 = c_j$ (j for "joint"). In each quadratic form we replace c_1 by c_j wherever it occurs, and we also replace c_6 by c_j wherever it occurs. The quadratic form marix will have one fewer row and column. It is constructed by *adding* rows 1 and 6 and also adding columns 1 and 6 together. If whole edges are to be identified, as in cylinder or torus boundary conditions, the rows for the pairs (triples, quartets) of vertices in the tesselaltion that are identified are to be combined by addition.

Example: A square $[0, 2\pi] \times [0, 2\pi]$ is to be mapped onto a torus. Divide the θ into 100 intervals with 101 points. Similarly for the ϕ direction. There will be a total of 101^2 vertices. The 99 interior vertices along both the θ and ϕ directions are pairwise identified and added, eliminating 2×99 rows and columns. The four vertices at $[0,0], [0,2\pi], [2\pi,0], [2\pi,2\pi]$ are identifed with a single point on the torus, squeezing four rows/columns down to one. The number of rows/columns in the matrices representing the quadratic forms for the Schrödinger equation on the torus is $101^2 - 2 \times 99 - (4-1) = 100^2$, as one would hope. The generalized eigenvalue equation then provides approximations to the solution on the boundary-free torus.

3.8 Scaling

Suppose we map a tessellated unit square into a torus. Assume the tessellation has 101 points per edge, and the torus has radii of the major and minor circles $a > b$. How do the energies/wavefunctions scale if we mapped the same square into a larger (smaller) torus whose length parameters are $\lambda a > \lambda b$?

Since length in the embedding scales like λ^2 and $\Delta x \to \lambda \Delta x$, the metric tensor g_{**} doesn't scale, nor does its inverse g^{**}. That means the kinetic energy $KE \simeq g^{**} \frac{\partial \psi}{\lambda \partial x^*} \frac{\partial \psi}{\lambda \partial x^*}$ scales like $1/\lambda^2$. Similarl;y, the curvatures scale like λ so the geometric potential scales like $1/\lambda^2$. As a result, the energies scale like $1/\lambda^2$.

Since the surfaace area scales like λ^2 and the output column vectors from the diagonaliztion are unchanges, these column vectors are mapped onto spacial

wavefunctions by multiplying by the vactor $1/\lambda^2$.

4 Examples

4.1 Ellipse

An ellipse in a plane can be parameterized in terms of an angle θ:

$$(x,y) = (a\cos\theta, b\sin\theta) \qquad \dot{\mathbf{x}} = (-a\sin\theta, b\cos\theta) \qquad \ddot{\mathbf{x}} = (-a\cos\theta, b\sin\theta) \tag{43}$$

The metric and curvature are

$$\begin{aligned} ds^2 = dx^2 + dy^2 = (a^2\sin^2\theta + b^2\cos^2\theta)(d\theta)^2 \Rightarrow g_{\theta\theta} = (a^2\sin^2\theta + b^2\cos^2\theta) \\ \kappa^2 = \frac{(a^2\sin^2\theta + b^2\cos^2\theta)(a^2\cos^2\theta + b^2\sin^2\theta) - (a^2-b^2)\sin\theta\cos\theta}{(a^2\sin^2\theta + b^2\cos^2\theta)^3} \end{aligned} \tag{44}$$

In particular,

$$\kappa_{(\pm a,0)} = \frac{a}{b^2} \qquad\qquad \kappa_{(0,\pm b)} = \frac{b}{a^2} \tag{45}$$

4.2 Ellipsoid

A triaxial ellipsoid is determined by the function

$$\frac{x^2}{a^2} + \frac{y^2}{b^2} + \frac{z^2}{c^2} = \text{cst.} \tag{46}$$

At any point (x,y,z) on this surface the normal is

$$\mathbf{N} \simeq (2x/a^2, 2y/b^2, 2z/c^2) \tag{47}$$

Unit vectors in the tangent plane at this point can be taken as

$$\mathbf{e}_1 = n_1\left(\frac{z}{c^2}, 0, -\frac{x}{a^2}\right) \qquad\qquad \mathbf{e}_2 = n_2\left(-\frac{xy}{a^2b^2}, \frac{x^2}{a^4} + \frac{z^2}{c^4}, -\frac{yz}{b^2c^2}\right) \tag{48}$$

where n_1, n_2 are appropriate normalization coefficients. The curvatures at (x,y,z) are obtained from Eq. (38):

$$K = \frac{\left\{ \begin{bmatrix} \frac{1}{a^2} & 0 & 0 \\ 0 & \frac{1}{b^2} & 0 \\ 0 & 0 & \frac{1}{c^2} \end{bmatrix} - \frac{\begin{bmatrix} \frac{x}{a^4} \\ \frac{y}{b^4} \\ \frac{z}{c^4} \end{bmatrix} \begin{bmatrix} \frac{x}{a^4} & \frac{y}{b^4} & \frac{z}{c^4} \end{bmatrix}}{\left(\left(\frac{x}{a^3}\right)^2 + \left(\frac{y}{b^3}\right)^2 + \left(\frac{z}{c^3}\right)^2\right)} \right\}}{\sqrt{(x/a^2)^2 + (y/b^2)^2 + (z/c^2)^2}} \tag{49}$$

The curvatures at the endpoints of the principal axes are

$$\kappa_{\pm a,0,0} = \frac{a}{b^2}, \frac{a}{c^2} \qquad \kappa_{0,\pm b,0} = \frac{b}{c^2}, \frac{b}{a^2} \qquad \kappa_{0,0,\pm c} = \frac{c}{a^2}, \frac{c}{b^2} \tag{50}$$

4.3 Tori

A recent theorem guarantees that every knot can be expressed as a "Chebyshev" knot: $\mathcal{K}(\theta) = (\cos a\theta, \cos b\theta, \cos c\theta + \psi)$ where a, b, c are relatively prime positive integers and ψ is some angle (0 or $\pi/2$ are the usual culprits). The first and second derivatives are

$$\begin{aligned} \dot{\mathcal{K}}(\theta) &= (-a\sin a\theta, -b\sin b\theta, -c\sin c\theta + \psi) \\ \ddot{\mathcal{K}}(\theta) &= (-a^2\cos a\theta, -b^2\cos b\theta, -c^2\cos c\theta + \psi) \end{aligned} \tag{51}$$

These are related to the tangent and normal vectors by $\hat{\mathbf{t}} = \dot{\mathcal{K}}(\theta)/|\dot{\mathcal{K}}(\theta)|$ and

$$\hat{\mathbf{n}} = \alpha\left(\ddot{\mathcal{K}}(\theta) - (\ddot{\mathcal{K}}(\theta)\cdot\hat{\mathbf{t}})\cdot\hat{\mathbf{t}}\right) \tag{52}$$

with α the normalization constant. Define the *binormal* $\hat{\mathbf{b}} = \hat{\mathbf{t}} \times \hat{\mathbf{n}}$. Then the torus $\mathcal{T}(\theta, \phi)$ surrounding the knot $\mathcal{K}(\theta)$ is defined by

$$\mathcal{T}(\theta, \phi) = \mathcal{K}(\theta) + a(\hat{\mathbf{n}}\cos\phi + \hat{\mathbf{b}}\sin\phi) \tag{53}$$

for a sufficiently small.

4.4 Surfaces Without Boundaries: Torus

The parameterization of a torus as described above involves mapping a square $0 \le \theta, \phi \le 2\pi$ onto the torus surface using the mapping described in Eq. (53). A tessellation of the square is easily made in the plane. This tessellation can be lifted to the torus with ease. However, there is a technical detail. Vertices at opposite sides of the square map to the same vertices on the torus.

To be explicit, suppose we represent vertices in the plane by (i_θ, i_ϕ), with i_θ and i_ϕ integers in the range $0 \le i_\theta, i_\phi \le 100$, so that the tessellation takes the form of intersecting horizontal and vertical lines. Each line will contain 101 vertices and the kinetic, potential, and overlap matrices will be $101^2 \times 101^2$. However, the two vertices $(0, i_\phi)$ and $(100, i_\phi)$ will map to the same vertex in the torus ($i_\phi \neq 0, 100$), and the four vertices $(0,0), (0,100), (100,0), (100,100)$ (the four corners of the square in the θ-ϕ plane) will all map to a single vertex in the torus. When this occurs the periodic boundary conditions are imposed as follows. If **a** and **b** are two vertices in the flat parameterizing plane that map to the same vertex in the torus, the row labeled **b** is added to the row labeled **a** and row **b** is eliminated. Ditto for columns. In this way the 99 rows $(i_\theta, 0)$ and $(i_\theta, 100)$, $0 < i_\theta < 100$ are consolidated. Similarly for $(0, i_\phi)$ and $(100, i_\phi)$. Finally, the contents of the three rows/columns $(0,100), (100,0), (100,100)$ of the kinetic, potential and overlap matrices are added to the contents of the row/column $(0,0)$ and removed. The resulting matrix has size $(101^2 - 2 \times 99 -$

3) $\times 100^2$. Solution of the generalized eigenvalue problem $(\mathcal{K} + \mathcal{V} - \lambda\mathcal{O})c = 0$ yields the values of the eigenstates ψ at the 100^2 vertices distributed over the torus. The periodic boundary conditions are enforced by this simple procedure.

4.4.1 Implementation

Creata a list of vertices that are to be identified, for example $[a, b, c]$ with $a < b < c$. There can be a complementary list of "independent" vertices: those that are not matched to others under periodic boundary conditions. Now create an $N_1 \times N_2$ matrix S of zeroes. N_1 is the number of vertices after the identification is made (*ex:* 100^2). Now start with the first list, and if $[a, b, c]$ is the first set of identifications in this list, overwrite a $+1$ in positions $(1, a), (1, b), (1, c)$. For the second member of this list go to the second column of S and overwrite the zeroes with 1 (*ex:* $(2, d), (2, e)$. Cointinue until the list of identified vertices is exhausted. Now go down the singlet list and place a $+1$ in the next column and appropriate row.

Then the mapping

$$H \to S^t H S = H' \tag{54}$$

converts the initial tessellation/computation to one satisfying the appropriate boundary conditions. When the smaller hamiltonian H' is diagonalized, the column vectors $[\psi(\alpha)]$ of length N_2 on the surface with periodic boundary conditions is converted (if desirable) to a column vector of length N_1 by multiplying by S. Doing this places the same amplitude at each of the vertices that are identified. Plotting over the initial tessellation than looks more continuous.

4.5 Genus-g

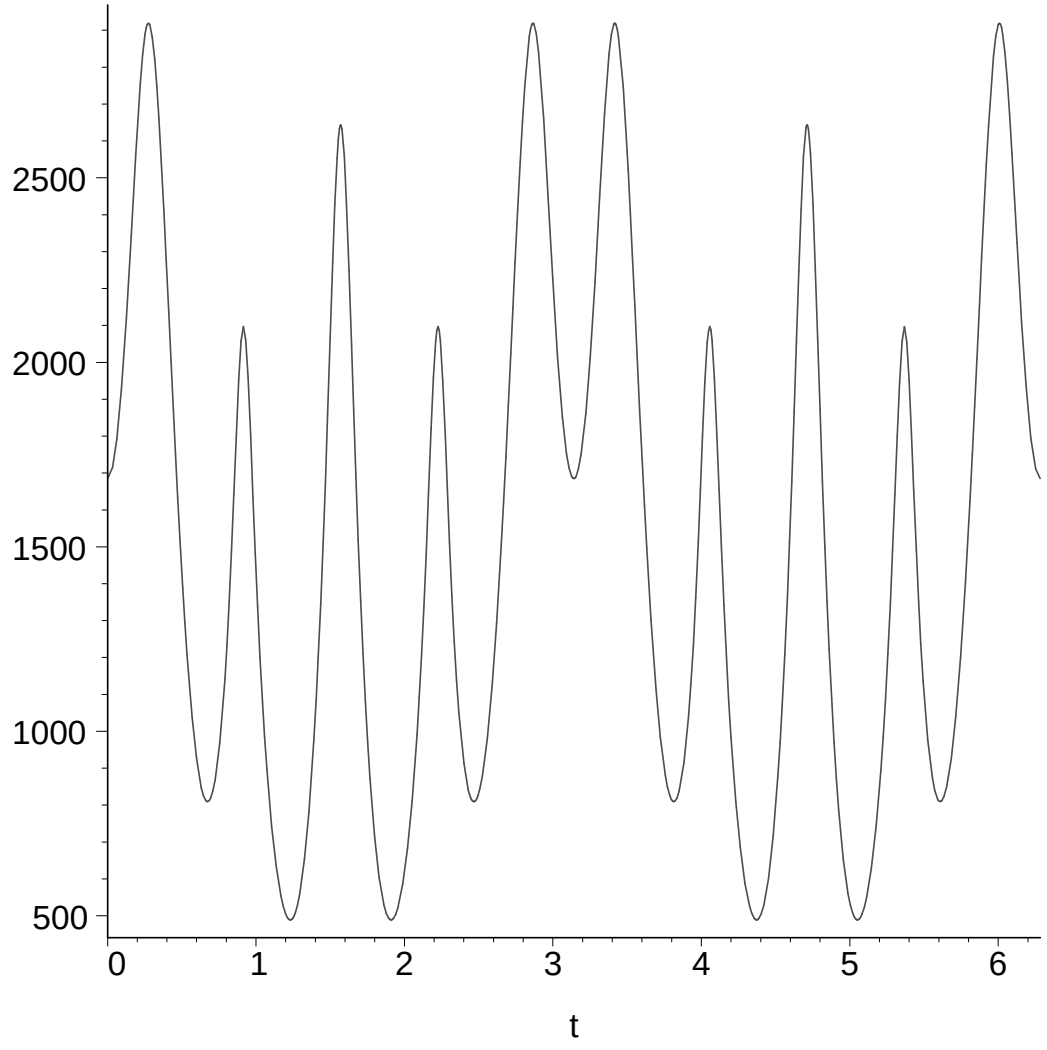
Any torus of genus $g > 1$ can be decomposed into unions of "trinions" (particle physics speak). The canonical decomposition contains $g - 1$ pairs of trinions, and each pair consists of a "joining" trinion and a "splitting" trinion (nonlinear dynamics-speak). In turn, each trinion can be decomposed into a pair of hexagons. Thus, a torus of genus g can be tessellated by $4(g-1)$ hexagons (see Fig. ?). Tessellating a hexagon is a piece of cake. Fig. ?? shows a hexagon tessellated with a hexagonal close packed lattice (solid state physics speak). If there are n equally spaced vertices per edge, the total number of vertices in the tessellation of each hexagon is $\mathrm{T} = 2\sum_n^{2n-1} k - (2n-1) = 3n^2 - 3n + 1$.

After 4 hexagons have been assembled into a genus-2 torus, the number of independent vertices, edges, and faces (v, e, f of dimensions 0, 1, 2) satisfy Euler's beautiful equality:

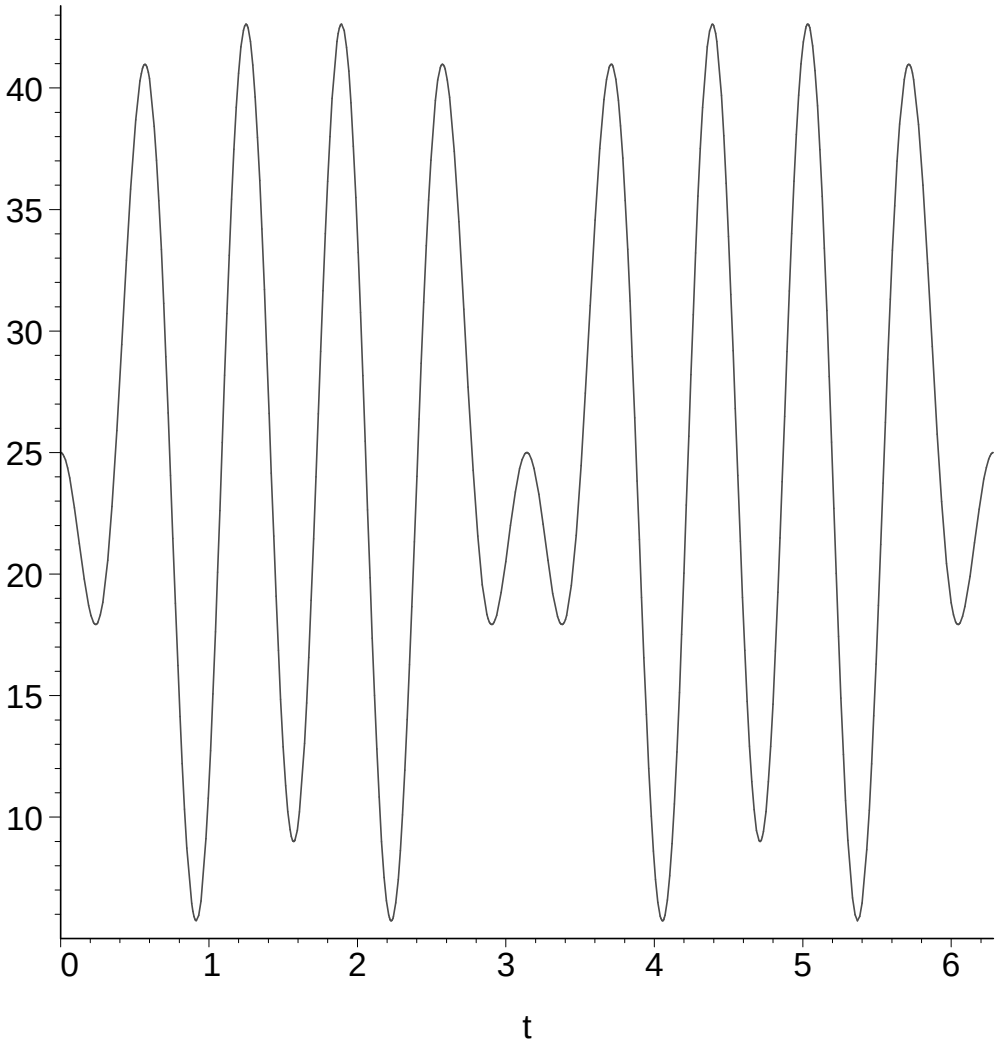
$$v - e + f = \chi(g = 2) = 2 - 2g = -2 \tag{55}$$

Every edge shares two faces and every face has three edges, so

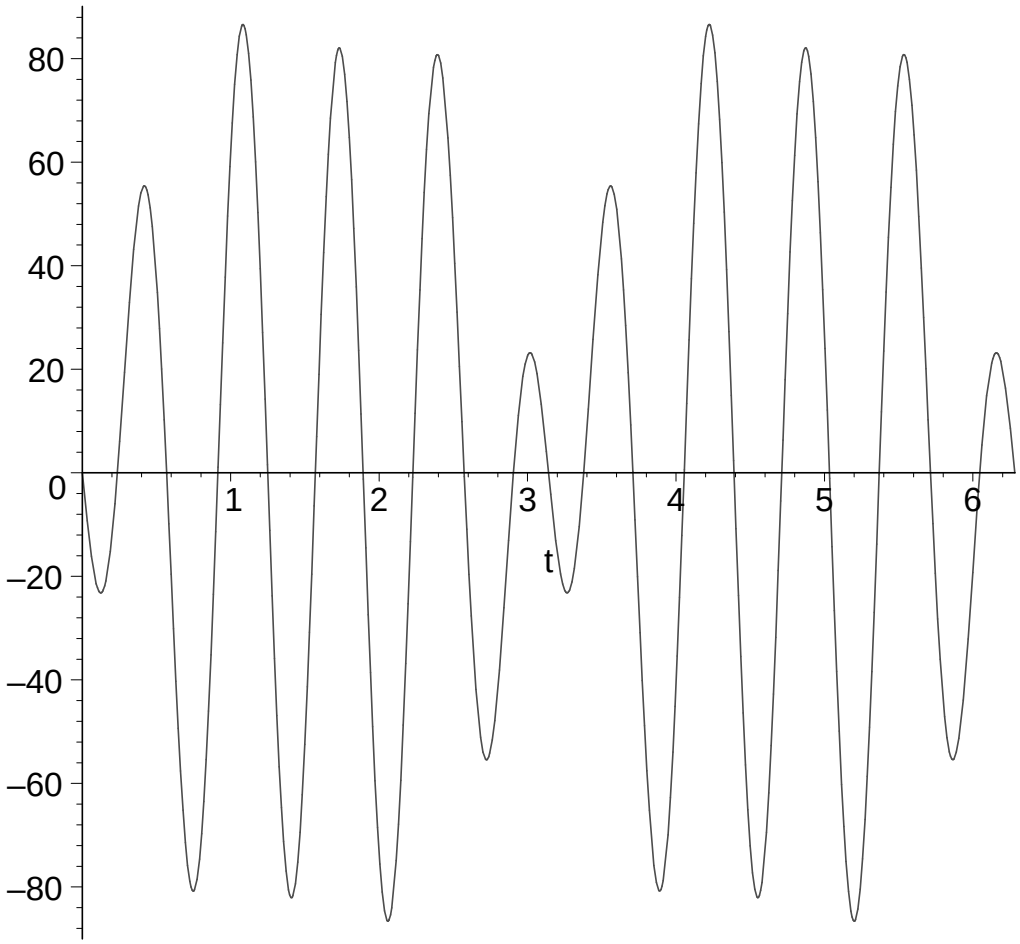
```
> a:=3:b:=4:c:=5:x0[1]:=cos(a*t):x0[2]:=cos(b*t):x0[3]:=cos(c*t+Pi/2
  ):
> for i from 1 to 3 do x1[i]:=diff(x0[i],t):x2[i]:=diff(x1[i],t):od:
> ip00:=x0[1]*x0[1]+x0[2]*x0[2]+x0[3]*x0[3]:
> ip11:=x1[1]*x1[1]+x1[2]*x1[2]+x1[3]*x1[3]:
> ip12:=x1[1]*x2[1]+x1[2]*x2[2]+x1[3]*x2[3]:
> ip22:=x2[1]*x2[1]+x2[2]*x2[2]+x2[3]*x2[3]:
> vgeom:=(ip11*ip22-ip12*ip12)/sqrt(ip11):
> plot(vgeom,t=0..2*Pi);
```



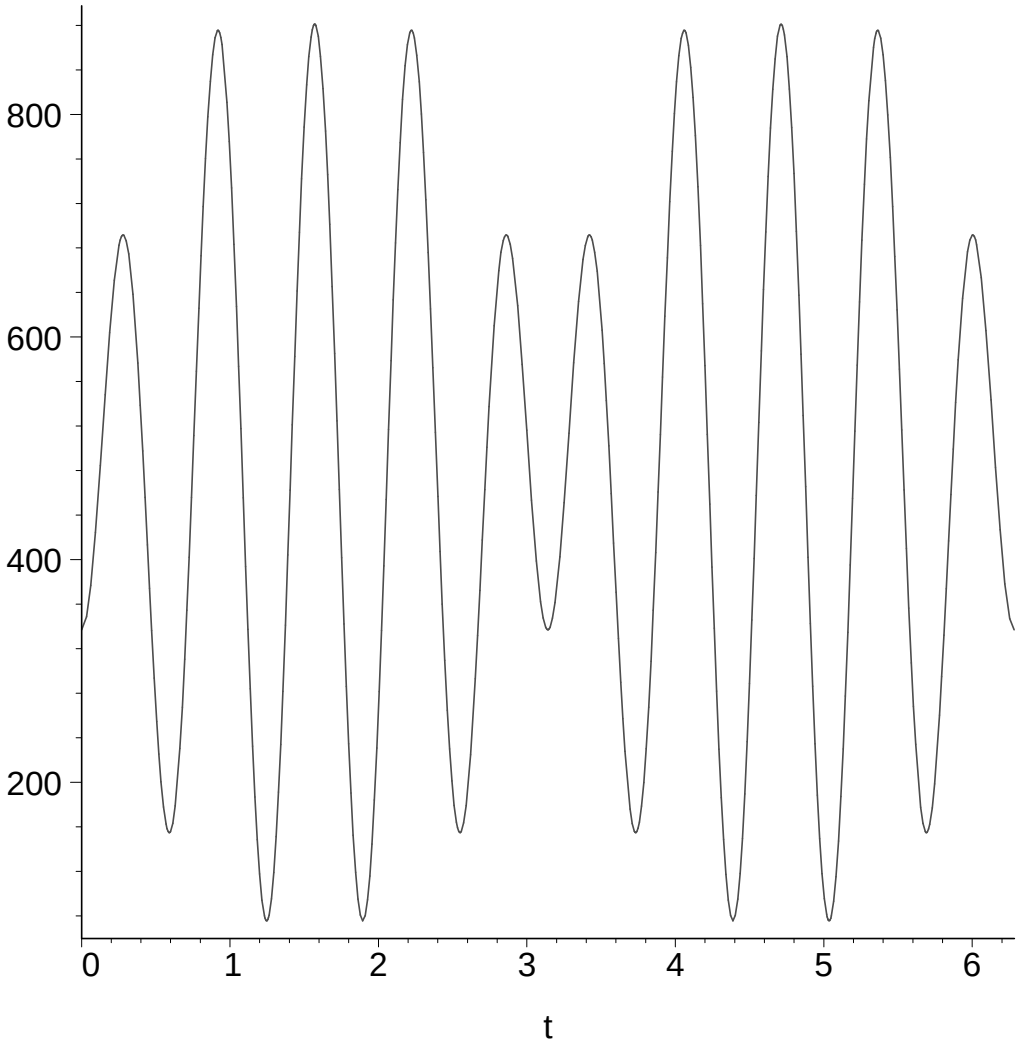

```
> plot(ip11,t=0..2*Pi);
```



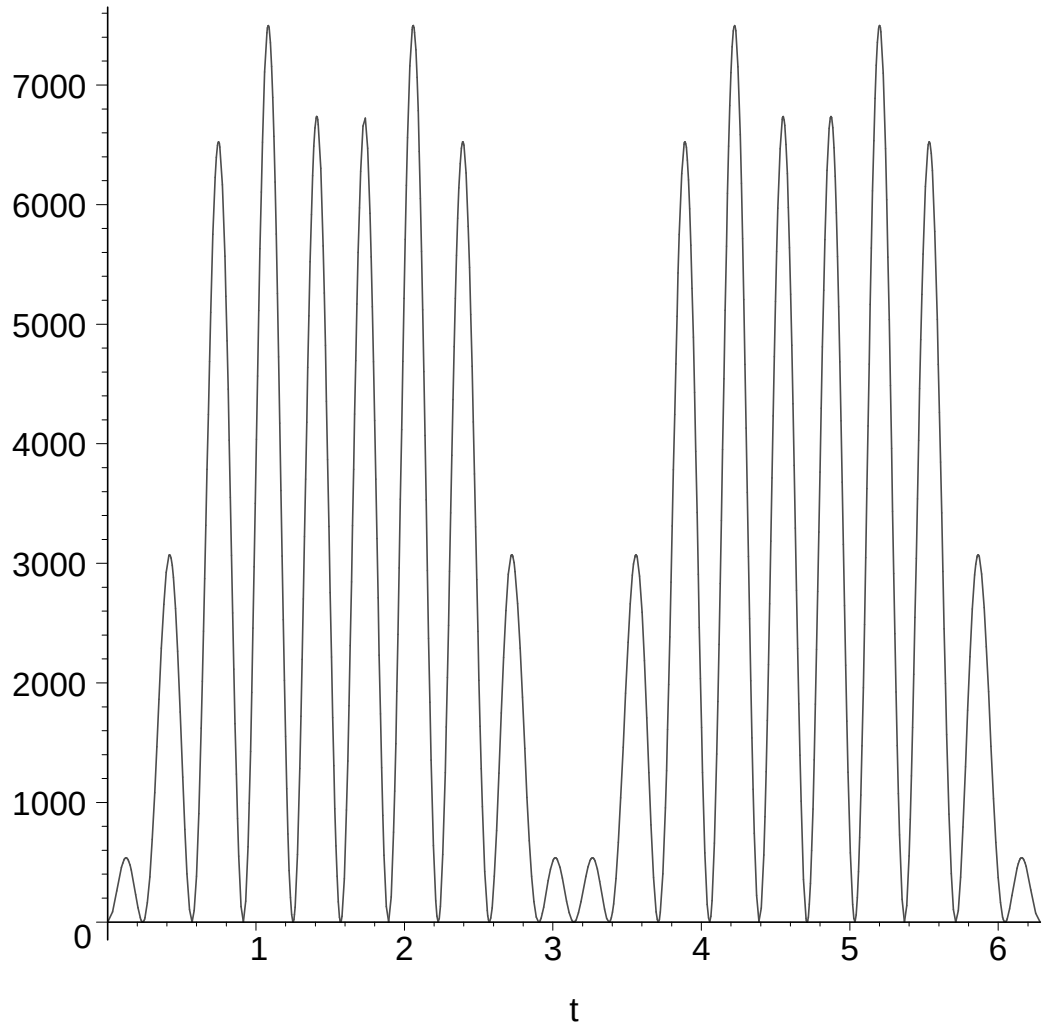

```
> plot(ip12,t=0..2*Pi);
```



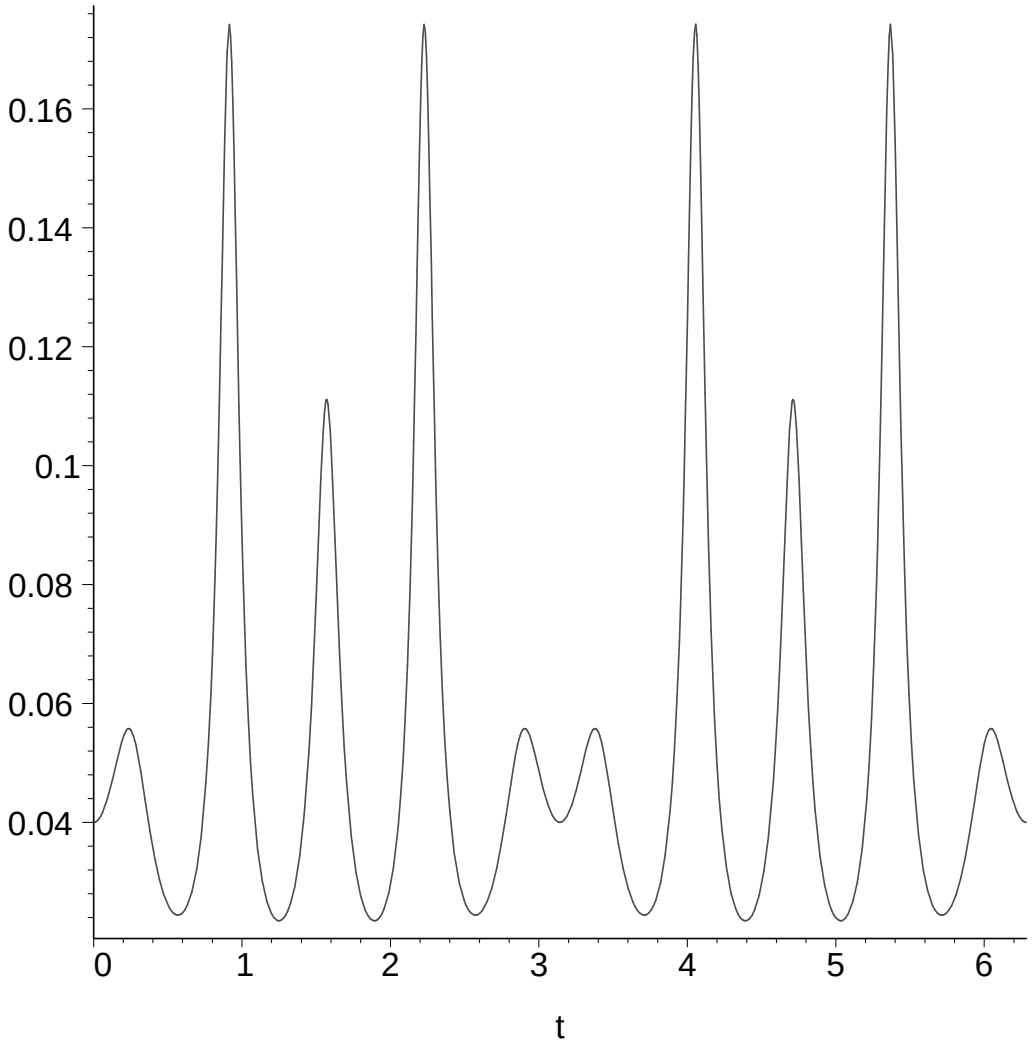

```
> plot(ip22,t=0..2*Pi);
```




```
> plot(ip12^2,t=0..2*Pi);
```




```
> plot(1/ip11,t=0..2*Pi);ke:=matrix(20,20);
```



ke := array(1 .. 20, 1 .. 20, [ ])

```
> 
> 
> 
> for i from 1 to 5 do  for j from 1 to 5 do
  ke[i,j]:=evalf(int(i*sin(i*t)*j*sin(j*t)/ip11,t=0..2*Pi));print(i,
  j,ke[i,j]):od:od:
```

1, 1, 0.1804363349

1, 2, $-0.1110423055\ 10^{-12}$

1, 3, 0.01301598313

1, 4, $0.1491545251\ 10^{-12}$

1, 5, -0.1941269700

2, 1, $-0.1110423055\ 10^{-12}$

2, 2, 0.7390999839

2, 3, $-0.1098290210\ 10^{-12}$

2, 4, -0.2758938636

2, 5, 0.

3, 1, 0.01301598313

3, 2, $-0.1098290210\ 10^{-12}$

3, 3, 1.313546418

3, 4, $0.3990922049\ 10^{-12}$

3, 5, -0.7093532830

4, 1, $0.1491545251\ 10^{-12}$

4, 2, -0.2758938636

4, 3, $0.3990922049\ 10^{-12}$

4, 4, 2.130337857

4, 5, 0.

5, 1, -0.1941269700

5, 2, 0.

5, 3, -0.7093532830

5, 4, 0.

5, 5, 5.531479229

```
> ###
> ###
> ###
> ###
> pe:=matrix(20,20):
> for i from 1 to 5 do for j from 1 to 5 do
  pe[i,j]:=evalf(-1*int(cos(i*t)*cos(j*t)*vgeom/4.0,t=0..2*Pi)):prin
  t(i,j,pe[i,j]):od:od:
```

1, 1, -1415.425823

1, 2, $-0.5852048669\ 10^{-11}$

1, 3, -361.8977670

1, 4, $-0.5931163371\ 10^{-11}$

1, 5, -109.3177836

2, 1, $-0.5852048669\ 10^{-11}$

2, 2, -1342.626940

2, 3, $-0.5887470617\ 10^{-11}$

2, 4, -182.1166668

2, 5, $-0.1743810662\ 10^{-9}$

3, 1, -361.8977670

3, 2, $-0.5887470617\ 10^{-11}$

3, 3, -1162.845839

3, 4, $-0.6013436116\ 10^{-11}$

3, 5, -261.7869334

4, 1, $-0.5931163371\ 10^{-11}$

4, 2, -182.1166668

4, 3, $-0.6013436116\ 10^{-11}$

4, 4, -1242.516106

4, 5, $-0.5952799506\ 10^{-11}$

5, 1, -109.3177836

5, 2, $-0.1743810662\ 10^{-9}$

5, 3, -261.7869334

5, 4, $-0.5952799506\ 10^{-11}$

5, 5, -901.6795583

>