Computer Science and Applied Mathematics

APPM2007 Lagrangian Mechanics

Tutorial 1

Question 1 (10 Points)

Methane is a chemical compound with the chemical formula CH_4 (one atom of carbon and four atoms of hydrogen). Methane is a tetrahedral molecule with four equivalent C-H bonds. Show that the angle subtended at the central Carbon atom by any two Hydrogen atoms in a methane molecule is 109.5°. (Hint: use the symmetry of the tetrahedron structure of the CH_4 molecule to aid your computations.)

Solution 1 (10 Points)

Consider the space \mathbb{R}^3 and place the atoms in the methane molecule in the following positions,

$$H \rightarrow p = (2,0,0)$$

 $H \rightarrow q = (0,2,0)$
 $H \rightarrow r = (0,0,2)$
 $H \rightarrow s = (2,2,2)$

$$C \to t = (1, 1, 1).$$

This positioning reproduces the tetrahedron shape of the methane molecule in \mathbb{R}^3 . The displacement vectors specifying the relative positions of each H atom relative to the central C atom are then

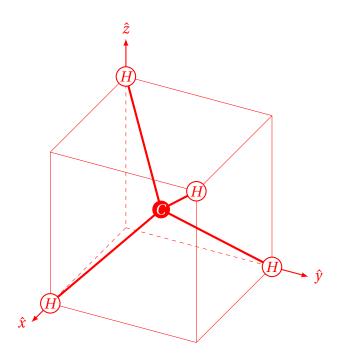
$$\vec{tp} = (1,-1,-1)$$

$$\vec{tq} = (-1, 1, -1)$$

$$\vec{tr} = (-1, -1, 1)$$

$$\vec{t}s = (1, 1, 1).$$

By symmetry under relabelling of the H atom placements relative to the position of the central C atom, we may consider any two vectors for consideration in the calculation to



follow, without loss of generality. Consider the vectors \vec{tp} and \vec{tp} . Clearly,

$$\|\vec{tp}\| = \|\vec{tq}\| = (-1, 1, -1) = \sqrt{3}$$

and

$$\vec{tp} \cdot \vec{tq} = -1$$
.

Recall that

$$\vec{tp} \cdot \vec{tq} = \|\vec{tp}\| \|\vec{tq}\| \cos(\theta)$$

such that

$$\cos(\theta) = \frac{\vec{t} p \cdot \vec{t} q}{\vec{t} p \cdot \vec{t} q} = -\frac{1}{3}.$$

Therefore,

$$\theta = \arccos\left(-\frac{1}{3}\right) = 109.47^{\circ} \approx 109.5^{\circ}.$$

Question 2 (5 Points)

Consider the space \mathbb{R}^2 . Compare the area element of the Rectilinear and Polar Co-ordinate systems on \mathbb{R}^2 . Do the Rectilinear and Polar Co-ordinate area elements co-incide?

Solution 2 (5 Points)

Consider the infinitesimal area element in each case for simplicity. Note that the magnitude of the area element of the rectilinear co-ordinate system is

$$\|\mathrm{d}\vec{a}\| = \mathrm{d}\|\vec{a}\| = \mathrm{d}a = \mathrm{d}x\,\mathrm{d}y,$$

where dx and dy are the extents of the infinitesimal area element in the \hat{x} - and \hat{y} -directions, respectively. Note that this area element has fixed magnitude everywhere in \mathbb{R}^2 , as such it is position independent. In polar co-ordinates, this becomes

$$\|\mathrm{d}\vec{a}\| = \mathrm{d}\|\vec{a}\| = \mathrm{d}a = \mathrm{d}r\,r\mathrm{d}\theta,$$

which is more commonly written as $da = rdr d\theta$, where dr is the extent of the infinitesimal area element in the \hat{r} -direction and $rd\theta$ is the extent of the same area element in the $\hat{\theta}$ -direction. Notice that this places a position dependence r on the magnitude of the area element in the polar co-ordinate system. Therefore, these area elements do not co-incide. \Box

Question 3 (10 Points)

Consider the plane \mathbb{R}^2 and the unit Sphere S^2 with north pole marked p. Construct the following co-ordinate mappings

- 1. $f: U \to S^2 \setminus \{p\}$ with $U \subset \mathbb{R}^2$ is finite. (Hint: use Riemann Normal Co-ordinates.)
- 2. $f: \mathbb{R}^2 \to S^2 \setminus \{p\}$. (Hint: use a co-ordinate projection where points in $c = \{z \in \mathbb{R}^2 : \|z\| \le 1\}$ are mapped to the southern hemisphere of S^2 and points outside c are mapped to the northern hemisphere of S^2 .)

Compare the qualitative differences and similarities of these two co-ordinatisation maps.

Solution 3 (10 Points)

To perform each of the following co-ordinatisations, it will be usefull to first embed S^2 in \mathbb{R}^3 to form a geometric description of the problem. In each construction it will be instructive to denote the radius of S^2 by R.

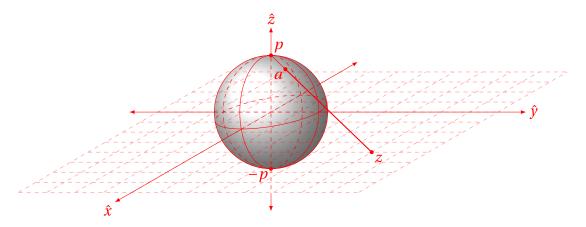
1. Introduce a system of Riemann Normal Co-ordinates (RNC) to S^2 by starting at point -p and then moving radially outward from -p towards the anti-podal point p. The radial distance l along the surface S^2 between -p and p is equal to half the diameter of S^2 ,

$$l = \pi R$$
.

A point z on any radial line connecting p and -p has radial position on the interval $[0,\pi R]$. Let $t\in[0,1]$ denote the fraction of the distance between -p and p occupied by z. Then the radial component of z is $Rt\pi$. Since this measures a fractional angular displacement, it is convenient to define $\theta=tR\pi$. The angular position of z corresponds to the angular displacement of z at fixed distance $0< c<\pi R$ from -p, from the initial radius line connecting -p to p. This measures an angle ϕ that is uniquely defined up to a multiple of 2π . Combining these radial and angular positions, with the assignment of R=1, we denote z by the co-ordinate pair (θ,ϕ) with $\theta\in[0,\pi]$ and $\phi\in[0,2\pi]$. This is a finite co-ordinitisation of S^2 . Additionally, the points -p and p have ambiguous descriptions with respect to ϕ . Each such point is called an *exceptional point*.

2. Intersect S^2 with \mathbb{R}^2 such that the equator lies on the unit circle in \mathbb{R}^2 . In this configuration, p = (0,0,R) and the line connecting p and -p intersects the plane at (0,0,0) and \mathbb{R}^2 corresponds to all points in \mathbb{R}^3 with z-co-ordinate equal to zero. Every line throught p meeting S^2 meets exactly one point in \mathbb{R}^2 , with the exception of lines tangent to S^2 at p. Choose a point $z = (r,s) \in \mathbb{R}^2$. This corresponds to a point

 $z=(r,s,0)\in\mathbb{R}^3$. The line passing through p and z intersects S^2 at some point a. This associates to each point $z\in\mathbb{R}^2$ a unique point $a\in S^2$. We call this association a *stereographic projection* (SP). Consider the figure below.



The line passing through z and a colinear with the vector

$$\vec{v} = (r, s, 0) - (0, 0, R) = (r, s, -R)$$

connecting p and z. Therefore the vector \vec{w} connecting p and a must originate at p and extend some distance along \vec{v} , so

$$\vec{w} = \vec{p} + \lambda \vec{w} = (\lambda r, \lambda s, R - \lambda).$$

The point *a* corresponds to the intersection of the line $(\lambda r, \lambda s, R - \lambda)$ with S^2

$$x^2 + y^2 + z^2 = R^2.$$

This gives an equation for λ

$$\lambda^{2} (r^{2} + s^{2} + R^{2})^{2} - 2\lambda = 0.$$

So,

$$\lambda = 0$$
 or $\lambda = \frac{2}{r^2 + s^2 + R^2}$.

Note that $\lambda = 0$ corresponds to the points $p \in S^2$ and the origin in \mathbb{R}^2 . For $\lambda \neq 0$, we have

$$a(r,s) = \left(\frac{2r}{r^2 + s^2 + R^2}, \frac{2s}{r^2 + s^2 + R^2}, \frac{r^2 + s^2 - R^2}{r^2 + s^2 + R^2}\right).$$

Recall that R = 1 on S^2 , so

$$a(r,s) = \left(\frac{2r}{r^2 + s^2 + 1}, \frac{2s}{r^2 + s^2 + 1}, \frac{r^2 + s^2 - 1}{r^2 + s^2 + 1}\right).$$

The number of parameters needed to identify a point $(r, s) \in \mathbb{R}^2$ now corresponds with the number of parameters needed to specify a(r, s). Note that this

co-ordinatisation also works at p, but corresponds to $r, s \to \infty$, which leads to an ambiguity in the description. Therefore, p is an exceptional point in this co-ordinatisation.

Each co-ordinate mapping contains at least one exceptional point, where the SP contains one fewer exceptional point than that of RNC at a cost of adding one extra dimension to the description. An interesting consequence of each mapping is that the RNC maintains a fixed scale over the whole sphere, while SP distorts the co-ordinate scale because the unit disc is mapped to the southern hemisphere of S^2 and the remainder of \mathbb{R}^2 is mapped to the northern hemisphere.

Question 4 (10 Points)

Consider a marked point in $p \in \mathbb{R}^3$. Let α , β and γ denote the angles subtended at the origin by the vector \vec{p} and each of the co-ordinate axes \hat{x} , \hat{y} and \hat{z} . Show that

$$\cos^2(\alpha) + \cos^2(\beta) + \cos^2(\gamma) = 1.$$

Solution 4 (10 Points)

Define the displacement vector starting at the origine of \mathbb{R}^3 and terminating at the point p=(a,b,c) as \vec{r} , and define \vec{x} , \vec{y} and \vec{z} as arbitrary length vectors directed along the positive co-ordinate directions. By these definitions, it is clear that,

$$\vec{r} = (a, b, c)$$

 $\vec{x} = (s, 0, 0)$
 $\vec{y} = (0, t, 0)$
 $\vec{z} = (0, 0, u)$.

Note that

$$\vec{r} \cdot \vec{r} = ||\vec{r}||^2 = a^2 + b^2 + c^2$$
.

For notational simplicity, denote $\|\vec{r}\| = r$. Similarly, it is clear that $\|\vec{x}\| = s$, $\|\vec{y}\| = t$ and $\|\vec{z}\| = u$. Then, from the dot product of \vec{r} with \vec{x} , \vec{y} and \vec{z} we recover the following relation among the projections of \vec{r} along each vector \vec{x} , \vec{y} and \vec{z} in terms of the internal co-ordinate representations of each vector,

$$\cos(\alpha) = \frac{\vec{r} \cdot \vec{x}}{\|r\| \|x\|} = \frac{as}{rs} = \frac{a}{r}$$
$$\cos(\beta) = \frac{\vec{r} \cdot \vec{y}}{\|r\| \|y\|} = \frac{bt}{rt} = \frac{b}{r}$$
$$\cos(\gamma) = \frac{\vec{r} \cdot \vec{z}}{\|r\| \|z\|} = \frac{cu}{ru} = \frac{c}{r}.$$

Notice that the angular cosines are independent of the scaling of the direction vectors \vec{x} , \vec{y} or \vec{z} . Clearly,

$$\cos^2(\alpha) + \cos^2(\beta) + \cos^2(\gamma) = \frac{a^2 + b^2 + c^2}{r^2} = \frac{r^2}{r^2} = 1.$$

Notice that this formulation made no prior assumptions of the specific direction or magnitude of \vec{r} or the magnitudes of the directional vectors \vec{x} , \vec{y} or \vec{z} and is therefore a more general statement that that implied by the original question.