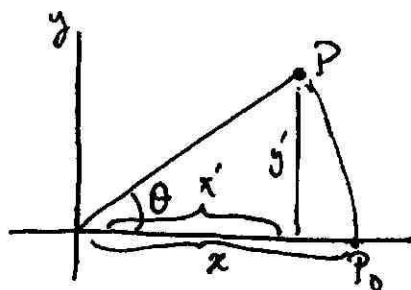


Problem Set 4-5

PV.1

1. Do problems 1-7 of the attached preliminary exam. This was the Chem 216 exam in Spring 2001. (It is the only prelim. I know of which is useful in preparing for the prelim I in this course.)

2. (i) Consider the point P generated from the point



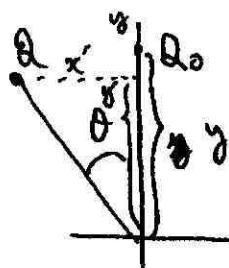
P_0 by rotation by the angle θ .

P_0 expressed as a column vector is $\begin{pmatrix} x \\ 0 \end{pmatrix}$ where the x refers to respectively the x & y axes.

The point P can be expressed as $\begin{pmatrix} x' \\ y' \end{pmatrix}$ (see picture), which converts $\begin{pmatrix} x \\ 0 \end{pmatrix}$

Find the matrix M_1 into $\begin{pmatrix} x' \\ y' \end{pmatrix}$ is in fact $M_1 = \begin{pmatrix} \cos\theta & \sin\theta \\ 0 & 1 \end{pmatrix}$ (ie, $M_1 \begin{pmatrix} x \\ 0 \end{pmatrix} = \begin{pmatrix} x' \\ y' \end{pmatrix}$)

(ii) Now consider the point Q



Find an M_2 similar to the M_1 previous example which has the property $M_2 \begin{pmatrix} 0 \\ y \end{pmatrix} = \begin{pmatrix} x' \\ y' \end{pmatrix}$

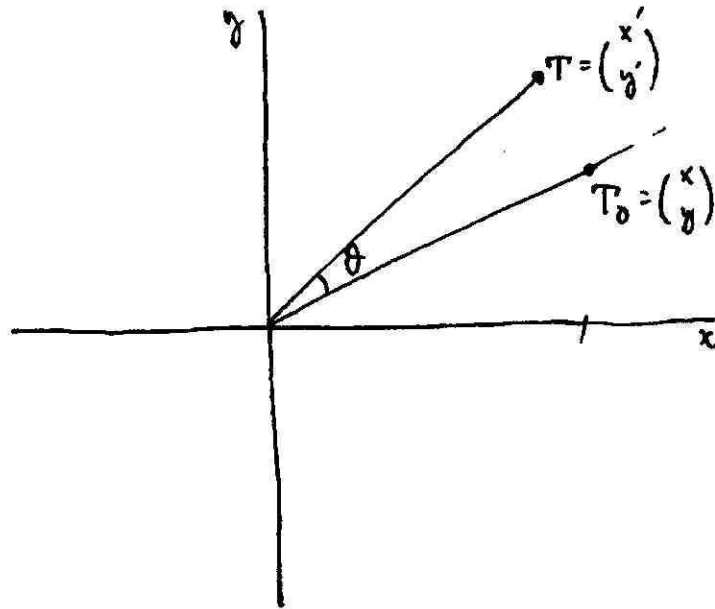
Problem Set -4-5

PV.2

(iii) Now consider a point T_0 . Rotate the point T_0 by the angle θ . If we call $\vec{T}_0 = \begin{pmatrix} x \\ y \end{pmatrix}$ & \vec{T} (the point after rotation $\begin{pmatrix} x' \\ y' \end{pmatrix}$), find R such that

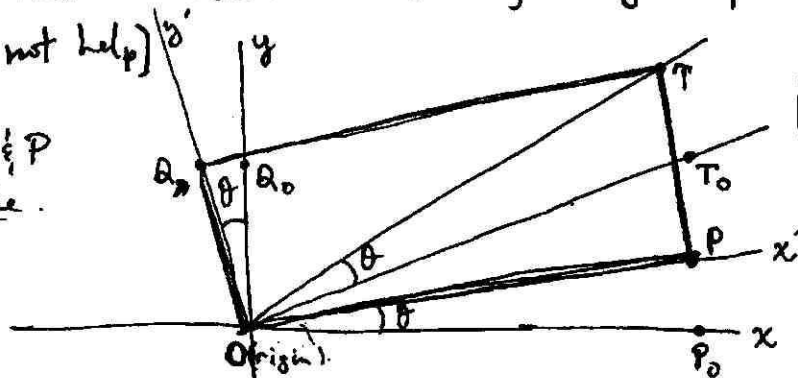
$$R\vec{T}_0 = \vec{T}$$

Express R as a function of only θ (R is a 2×2 matrix)



To find the answer the following picture may help (it may not help)

Note T, Q_0, O & P form a rectangle.



So knowing P & Q_0 we can figure out T

The matrix R is sometimes called the rotation matrix which goes from the x, y coordinate position to the x', y' coordinate position. Why is that so?

3. According to Zundahl (p.538)

$$\psi_{1s} = \frac{1}{\sqrt{\pi}} \left(\frac{z}{a_0} \right)^{3/2} e^{-\sigma}$$

$$\psi_{2p_z} = \frac{1}{4\sqrt{2}\pi} \left(\frac{z}{a_0} \right)^{3/2} \sigma e^{-\sigma/2} \cos\theta$$

where $z=1$ for hydrogen & a_0 & σ are defined in Zundahl.

For a hydrogen atom find the relative probability an electron is located at $(r = 5.29 \times 10^{-11} \text{ m}, \theta = 0, \phi = 0)$ for the following 3 wavefunctions:

$$\psi_{1s}, \psi_{2p_z}, \frac{1}{\sqrt{2}}(\psi_{1s} + \psi_{2p_z})$$

4. Multiply the following matrices and vectors

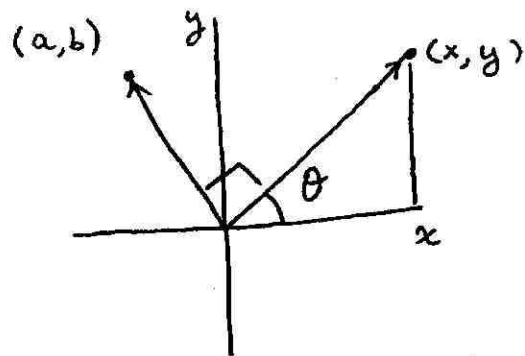
(i) $(\cos\theta, -i\sin\theta) \begin{pmatrix} \cos\theta \\ i\sin\theta \end{pmatrix}$

(ii) $\begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}$

(iii) $\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$

(iv) $\begin{pmatrix} \cos\theta & -\sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}$

5. Orthogonality of vectors.



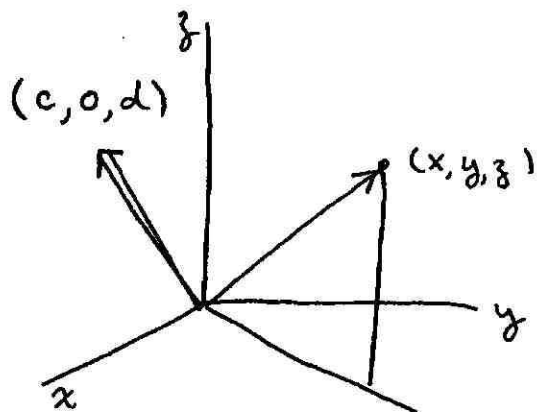
Consider a vector (a, b) which is perpendicular to another vector (x, y)

Express (a, b) in terms of x & y .

$$\text{Show } (a, b) \begin{pmatrix} x \\ y \end{pmatrix} = 0$$

Two vectors whose dot product is zero are said to be orthogonal. Geometrically they are \perp to each other.

6. Consider now a 3-D case.



Find a vector $(c, 0, d)$ which is perpendicular to the vector (x, y, z) .