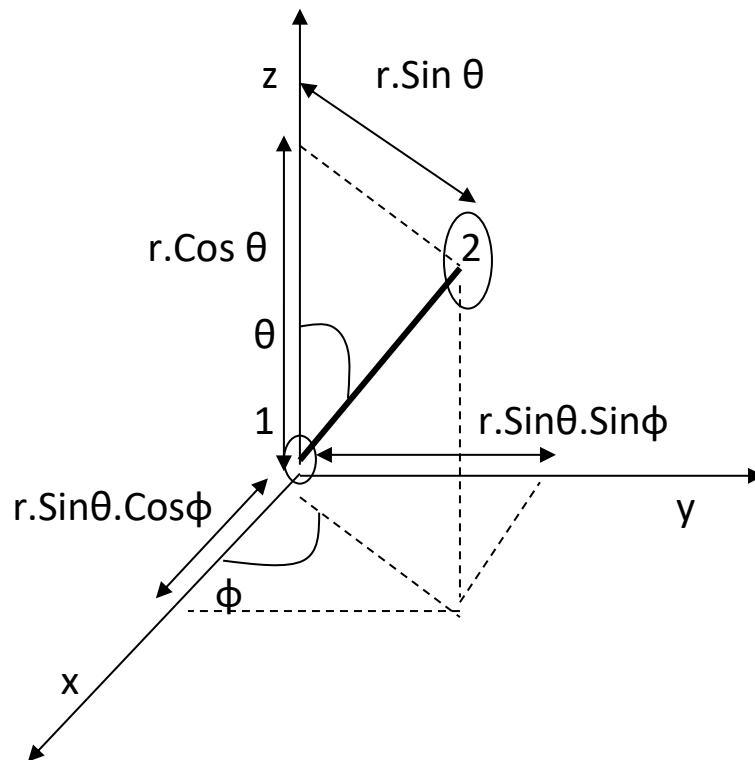


REDUCED MASS IN THE ENERGY EXPRESSION OF A RIGID ROTOR:

Figure 1.1



We see that when transcribing into polar coordinates

$\hat{H} = -(\hbar^2 / 2m)\nabla^2 + V(r)$ negative sign it is because the E_t be negative

$(-i = -\sqrt{-1}, i^2 = -1)$.

When at the center of gravity of the rigid rotor I will say that its center of mass is : $X_{cm} = m_1.x_1 / (m_1 + m_2) + m_2.x_2 / (m_1 + m_2)$

Same with Y_{cm} and Z_{cm} in the case of 2-D or 3-D.



$$x_2 - x_1 = r \cdot \sin\theta \cdot \cos\phi$$

$$y_2 - y_1 = r \cdot \sin\theta \cdot \sin\phi$$

$$z_2 - z_1 = r \cdot \cos\theta$$

We find from the equation Schrödinger that

$$\nabla^2\Psi + V(r)\Psi = E \cdot \Psi$$

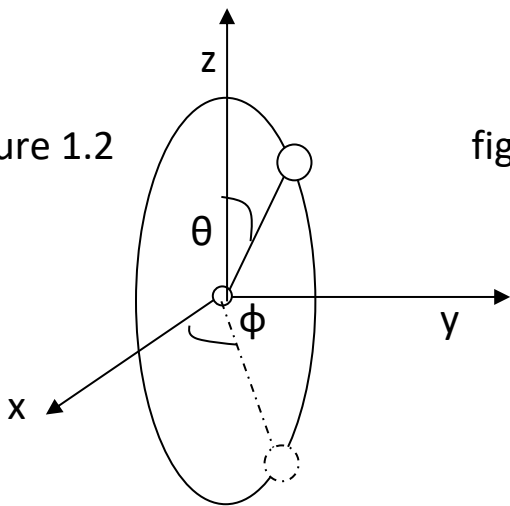
E = translation part + rotation part + vibration part

$$\text{that is : } E = \frac{1}{2}(m_1 + m_2)(\dot{x}^2 + \dot{y}^2 + \dot{z}^2) + \frac{1}{2}\left(\frac{m_1 \cdot m_2}{m_1 + m_2}\right)$$

$$[\dot{r}^2 + r^2 \cdot \dot{\theta}^2 + (\sin^2\theta \cdot \dot{\phi}^2)] + V(r) \quad (\text{figure 1.1})$$

In the case of the rigid rotor only 2 rotations fit (the 3rd ^{was} it is about itself therefore it is not considered)

figure 1.2

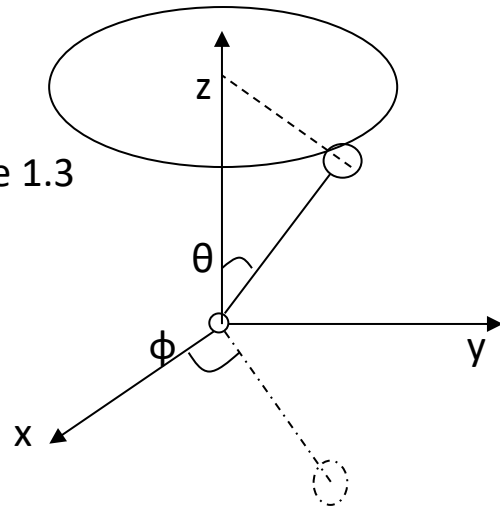


where z varies and,

otherwise θ

while ϕ remains constant

figure 1.3



therefore, θ also

remains

constant and ϕ varies (obviously x and y also).

remembering the following inequalities :

$\|\vec{a}\vec{b}\| \leq \|\vec{a}\| \cdot \|\vec{b}\|$ and $\|\vec{a}+\vec{b}\| \leq \|\vec{a}\| + \|\vec{b}\|$ we can assimilate them

Pythagorean theorem since in figure 1 everything they are triangles rectangles . Then we first derive and then we square it :

fig. 1.2:

$$c_{\dot{\theta}} = r \cdot \cos \theta + r \cdot \sin \theta$$

Now we derive where the variable is θ : $r \cdot \cos \theta \cdot \dot{\theta} + r \cdot \sin \theta \cdot \dot{\theta}$

And now we square it since we we find with a triangle rectangle :

$$c_{\dot{\theta}}^2 = r^2 \cdot \cos^2 \theta \cdot \dot{\theta}^2 + r^2 \cdot \sin^2 \theta \cdot \dot{\theta}^2$$

since and $\cos^2 \theta + \sin^2 \theta = 1$ we obtain: $c_{\dot{\theta}}^2 = r^2 \cdot \dot{\theta}^2$

Likewise when x and y vary : only we will derive with respect to ϕ and we will also use the resource of the previous Pythagorean theorem , therefore we will obtain :

$$C_{\text{tnt}} = r \cdot \sin \theta \cdot \sin \phi + r \cdot \sin \theta \cdot \cos \phi$$

now we derive where the variable is ϕ :

$$\dot{C}_{\text{tnt}} = r \cdot \sin \theta \cdot \cos \phi \cdot \dot{\phi} - r \cdot \sin \theta \cdot \sin \phi \cdot \dot{\phi}$$

being a triangle rectangle ,

$$\dot{C}_{\text{tnt}}^2 = r^2 \cdot \sin^2 \theta \cdot \sin^2 \phi \cdot \dot{\phi}^2 + r^2 \cdot \sin^2 \theta \cdot \cos^2 \phi \cdot \dot{\phi}^2$$

Where $\sin^2 \phi + \cos^2 \phi = 1$, that is, by the same procedure we are left with $r^2 \cdot \sin^2 \theta \cdot \dot{\phi}^2$ (figure 1.3)

As a consequence we see that figure 1.2 and 1.3 are inscribed in figure 1.1.