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Elliptical Coordinates

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Elliptical Coördinates
ellip_coord.tex

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I. SYNOPSIS

The Cartesian coördinate system and the spherical polar one are familiar to most students, but the elliptical coördinate system is so unfamiliar that a "tutorial" on it is appropriate. Since the H_2^+ system, the prototypical molecule (although without electron pair bonding), most easily is treated in this coördinate scheme, chemists have a vested interest in learning how to deal with it.

If r_A is the distance from nucleus A to a point P(x,y,z) (where the electron is located, in H_2^+, presumably), and r_B is the distance from nucleus B to the same point(!), then Elliptical Coordinates are defined as:

$$\lambda \equiv \frac{r_A + r_B}{R}$$

and

$$\mu \equiv \frac{r_A - r_B}{R}$$

(where ϕ is the same as the coordinate used in Spherical Polar Coordinates), which means that, adding,

$$r_A = \frac{R}{2}(\lambda + \mu)$$

and subtracting,

$$r_B = \frac{R}{2}(\lambda - \mu)$$

This also means that, by elementary geometry,

$$r_A = \sqrt{x^2 + y^2 + (z - R/2)^2}$$

and

$$r_B = \sqrt{x^2 + y^2 + (z + R/2)^2}$$

We seek the transformation equations between (x,y, and z) on the one hand and (λ, μ, ϕ) on the other.

To start, we write

$$r_A^2 = \left(\frac{R}{2}\right)^2 (\lambda + \mu)^2 = x^2 + y^2 + (z - R/2)^2 = x^2 + y^2 + z^2 - 2zR/2 + \left(\frac{R}{2}\right)^2 \tag{1.1}$$

i.e.,

$$r_A^2 = r^2 - 2zR/2 + \left(\frac{R}{2}\right)^2$$

and

$$r_B^2 = \left(\frac{R}{2}\right)^2 (\lambda - \mu)^2 = x^2 + y^2 + (z + R/2)^2 = x^2 + y^2 + z^2 + 2zR/2 + \left(\frac{R}{2}\right)^2 \tag{1.2}$$

i.e.,

$$r_B^2 = r^2 + 2zR/2 + \left(\frac{R}{2}\right)^2$$

so that (adding Equations 1.1 and 1.2)

$$r_A^2 + r_B^2 = 2\left(x^2 + y^2 + z^2 + \left(\frac{R}{2}\right)^2\right) = 2\left(\lambda^2 + \mu^2\right)\left(\frac{R}{2}\right)^2 = 2r^2 + 2\left(\frac{R}{2}\right)^2$$

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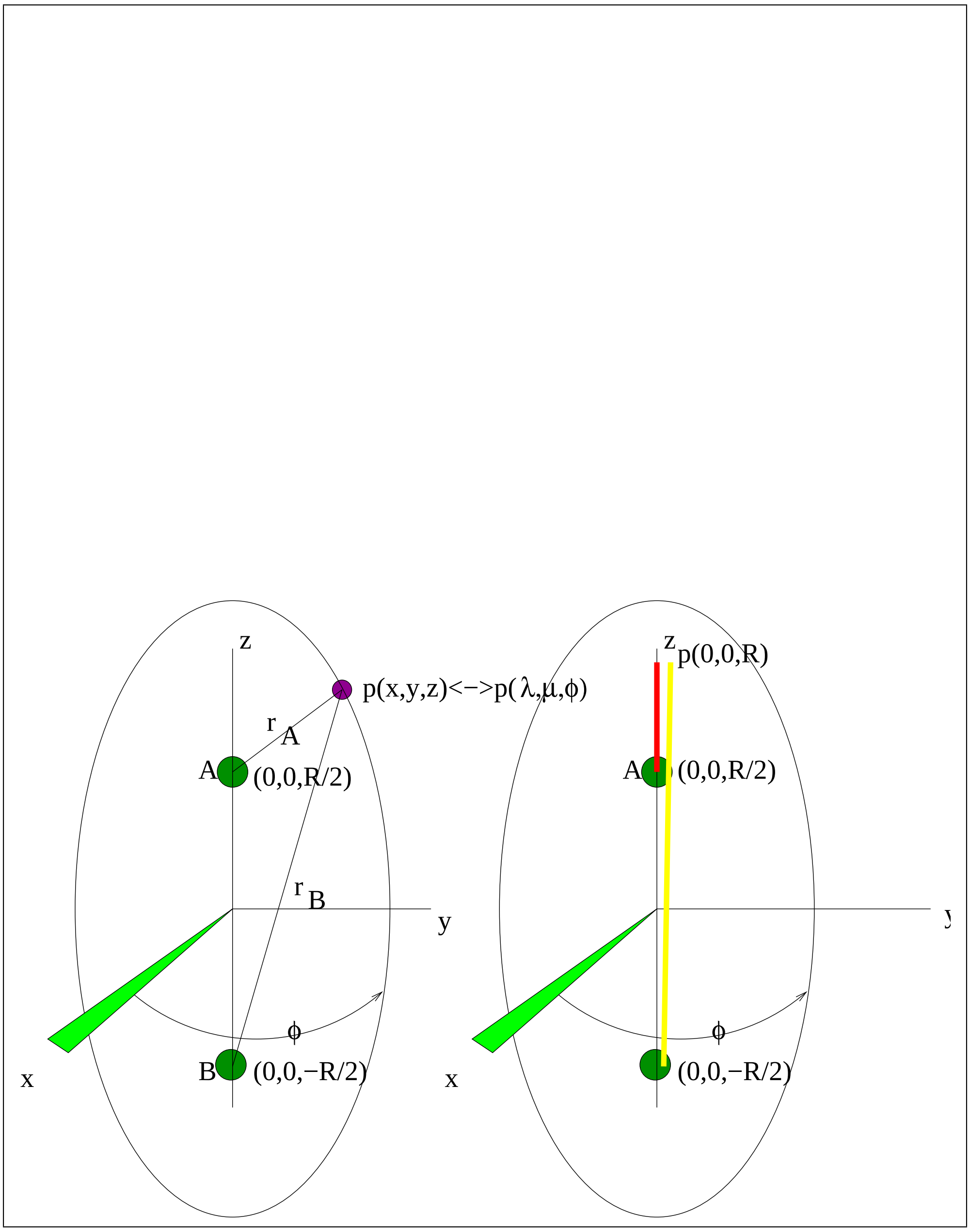

FIG. 1: The Elliptical Coordinate System for Diatomic Molecules. The ellipse is the locus of constant λ. The μ coordinate is not depicted. On the right hand side, one sees the depiction of the point (0,0,R) which would make r_A=R/2 and r_B=3R/2

so

$$r^2 = \left(\lambda^2 + \mu^2\right)\left(\frac{R}{2}\right)^2 - \left(\frac{R}{2}\right)^2$$

and

$$r^2 = \left(\frac{R}{2}\right)^2 \left(\lambda^2 + \mu^2 - 1\right) \tag{1.3}$$

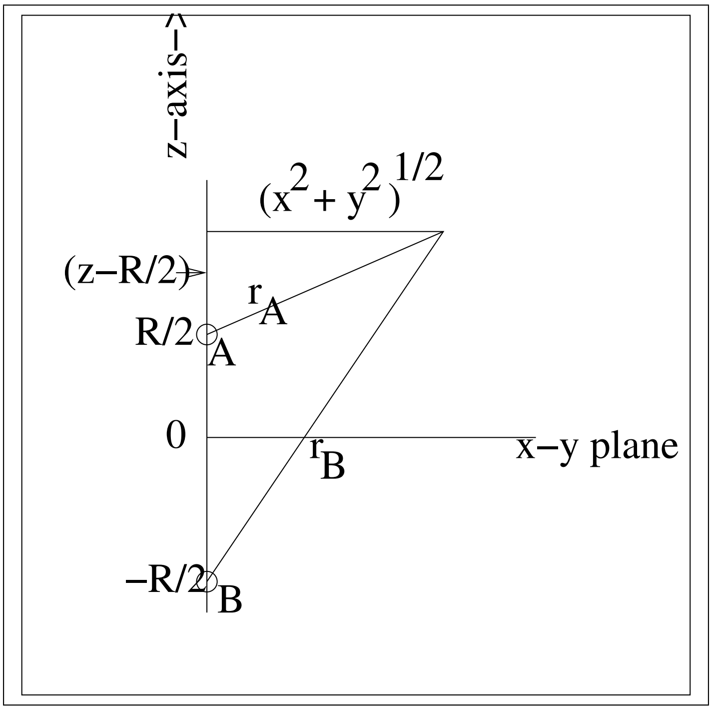

FIG. 2: The Elliptical Coordinate System for Diatomic Molecules. The construction of the triangle defining r_A is shown. A similar triangle based on $z+R/2$ is used to obtain r_B.

We need the z-coordinate first, so, subtracting Equation 1.2 from Equation 1.1 instead of adding, we obtain

$$(z-R/2)^2-(z+R/2)^2=\frac{R^2}{4}\left((\lambda+\mu)^2-(\lambda-\mu)^2\right)=\left(\frac{R}{2}\right)^2\left(\lambda^2+2\lambda\mu+\mu^2-(\lambda^2-2\lambda\mu+\mu^2)\right)$$

i.e.,

$$-4z\frac{R}{2}=\left(\frac{R}{2}\right)^2(4\lambda\mu)$$

or

$$z=-\frac{R\lambda\mu}{2} \quad (1.4)$$

This is our first transformation equation. To check that this is correct, we examine the point (0,0,R) which would have r_A=R/2 and r_B=3R/2 as shown in the diagram. From Equation 1.4 we have

$$R=-\frac{R}{2}\lambda\mu=-\frac{R}{2}\frac{1}{R}(R/2+3R/2)\frac{1}{R}(R/2-3R/2)$$

which is

$$R=-\frac{1}{2R}(2R)(-R)$$

We return now to obtaining x and y in this new coordinate system. Since, in spherical polar coordinates one has

$$\cos\theta=\frac{z}{r}$$

it follows that

$$\sin^2\theta=1-\cos^2\theta=1-\left(\frac{z}{r}\right)^2$$

i.e,

$$r\sin\theta=r\sqrt{1-\left(\frac{z}{r}\right)^2}=\sqrt{r^2-z^2}$$

Using Equation 1.4, we have

$$r\sin\theta=\sqrt{r^2-\left(\frac{R\lambda\mu}{2}\right)^2}$$

and (using Equation 1.3)

$$r\sin\theta=\sqrt{\left(\frac{R}{2}\right)^2(\lambda^2+\mu^2-1)-\left(\frac{R\lambda\mu}{2}\right)^2}$$

i.e.,

$$r \sin\theta = \frac{R}{2}\sqrt{(\lambda^2 + \mu^2 - 1 - \lambda\mu)}$$

then

$$x = r \sin\theta \cos\phi$$

i.e.,

$$x = \frac{R}{2}\cos\phi\sqrt{(\lambda^2 - 1)(1 - \mu^2)}$$

and

$$y = \frac{R}{2}\sin\phi\sqrt{(\lambda^2 - 1)(1 - \mu^2)}$$

II. SYNOPSIS

For future reference, we collect the transformation equations here:

$\lambda = \frac{r_A + r_B}{R}$	$x = \frac{R}{2}\cos\phi\sqrt{(\lambda^2 - 1)(1 - \mu^2)}$
$\mu = \frac{r_A - r_B}{R}$	$y = \frac{R}{2}\sin\phi\sqrt{(\lambda^2 - 1)(1 - \mu^2)}$
$\phi = \phi$	$z = -\frac{R\lambda\mu}{2}$