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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

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

i.e.,

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

and

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

i.e.,

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

so that (adding Equations 1.1 and 1.2)

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

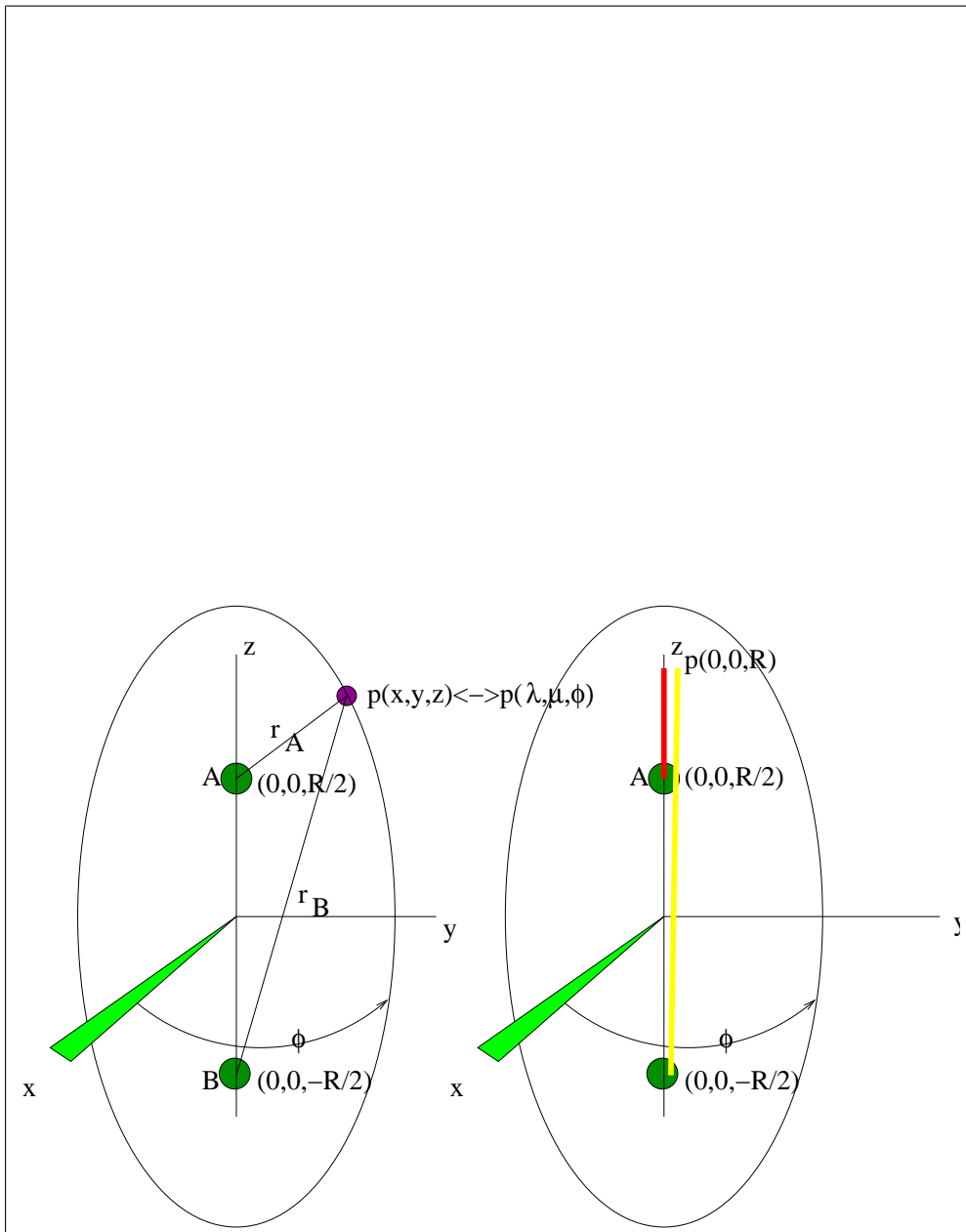


FIG. 1: The Elliptical Coordinate System for Diatomic Molecules. The ellipse is the locus of constant λ . The μ coordinate is not depicted. On the right hand side, one sees the depiction of the point $(0,0,R)$ which would make $r_A=R/2$ and $r_B=3R/2$

so

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

and

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

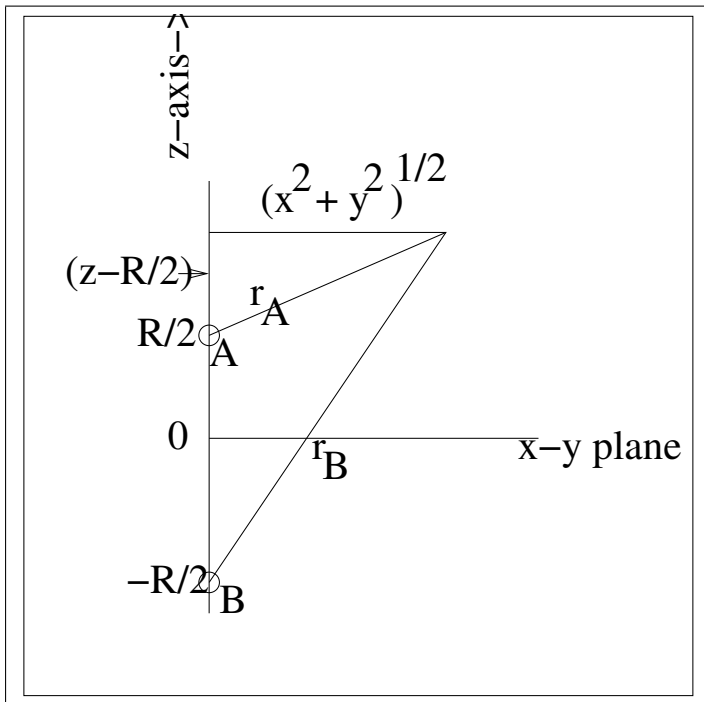


FIG. 2: The Elliptical Coordinate System for Diatomic Molecules. The construction of the triangle defining r_A is shown. A similar triangle based on $z + R/2$ is used to obtain r_B .

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

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

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:

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