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Understanding Atomic (Hydrogenic) Hybrid Orbitals Part 2, sp^2

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I. SYNOPSIS

This is a continuation of the discussion of hybrid orbitals, this time focussing on sp^2 orbitals, the last of the sets which can be plotted easily on a piece of paper.

II. INTRODUCTION

We here address them with sp^2 orbitals. They are combinations of a $2s$ orbital and two $2p$ orbitals, $2p_x$ and $2p_y$. The $2p_z$ orbital is normally reserved for use in π bonding, which is another topic.

III. NORMALIZATION

We show, in the attached Maple code, that the normalization constants for the $2s$ and $2p$ orbitals that contribute herein are the same, and therefore ignorable (from our point of view of plotting them).

IV. sp^2 ORBITALS

We start with an s and two p orbitals. The standard choice involves using p_x and p_y orbitals. We arbitrarily choose to keep the p_z orbital by itself (often used to form π bonds, but that's another story) [1].

$$\psi_{sp_1^2} = \frac{1}{\sqrt{3}}\psi_{2s} + \sqrt{\frac{2}{3}}\psi_{2p_x} + 0\psi_{2p_y}$$

and

$$\psi_{sp_2^2} = \frac{1}{\sqrt{3}}\psi_{2s} - \frac{1}{\sqrt{6}}\psi_{2p_x} + \frac{1}{\sqrt{2}}\psi_{2p_y}$$

Note that we do not use a $1s$ orbital!

The $2s$ hydrogenic orbital has the form

$$\psi_{2s} = (2 - r)e^{r/2}$$

where we are still assuming an atomic charge of 1 (we could assume a carbon like value, but would learn almost nothing from it, so why bother?). The p_z orbital has the form

$$\psi_{2p_x} = r \sin \vartheta \cos \varphi e^{r/2}$$

$$\psi_{2p_y} = r \sin \vartheta \sin \varphi e^{r/2}$$

as usual.

In Cartesian coördinates we have

$$\psi_{sp_1^2} = \left((2 - \sqrt{x^2 + y^2 + z^2}) + z \right) e^{\sqrt{x^2 + y^2 + z^2}/2}$$

How are we to understand this orbital, as given?

V. A NON-TRADITIONAL PLOT

Let's do what we did with simple hydrogenic orbitals, i.e., plot $\psi_{sp^+}(x, 0, z)$ versus x and z . We see that there

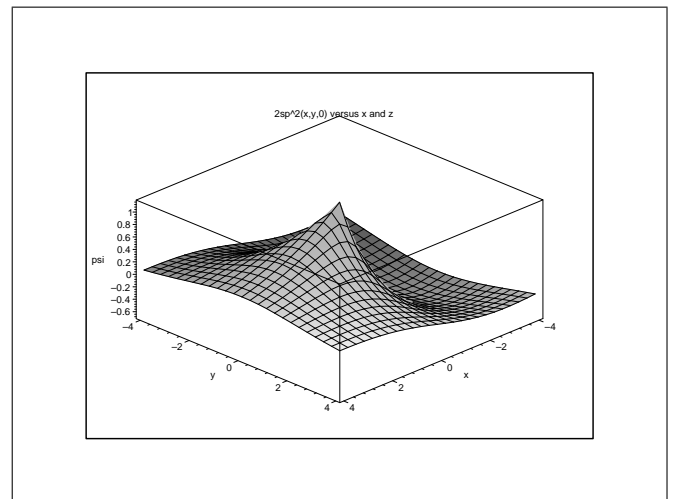


FIG. 1: The pseudo 3D surface of $\psi(x, 0, z)$ versus x and y . Notice the captioning error.

is a positive peak somewhere in the region $z > 0$. There is a valley (negative) appearing on the negative z axis. Both of these features tail off as $|x|$ grows.

VI. A CONTOUR PLOT

We next create a contour plot of $\psi_{sp^2}(x, y, 0)$ versus x and y in two dimensions. This is Figure 2, a plot showing loci of constant ψ .

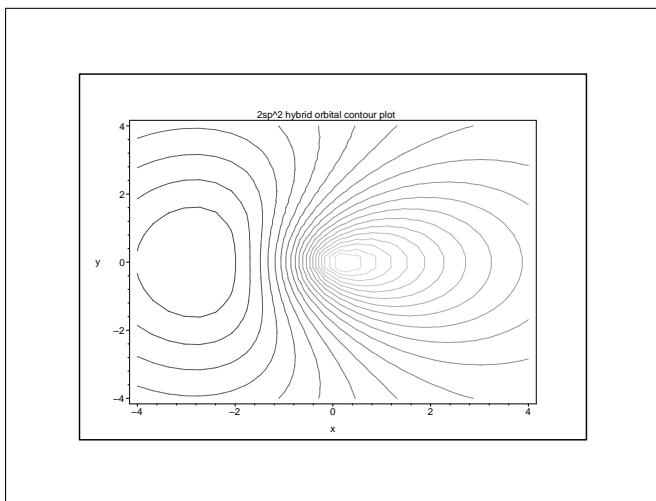


FIG. 2: A contour map of $\psi(x, y, 0)$ with x and y

VII. NON-TRADITIONAL PLOTS

Now, we want to look a little more at this function. First, we re-write it as

$$\psi_{sp_1^2} = ((2 - r) + r \sin \vartheta \cos \varphi) e^{r/2}$$

and fix the value of r at some (arbitrary) value, say “1”. Then, ignoring the exponential, we have

$$\psi_{sp_1^2} = ((2 - 1) + 1 \sin \vartheta \cos \varphi) e^{r/2}$$

and we now set $\vartheta = \frac{\pi}{2}$ so that we are “in the x - y plane. this allows us to make a polar plot of this function ($1 + \cos \varphi$) in the traditional manner. We eschew this here, since we’ve done it before for the sp case.

Instead, we construct the 3-dimensional contour plot in x , y , and z space in Figure 3. Notice that this is really two plots, one for the positive lobe, the other for the negative one, superimposed.

VIII. ANOTHER sp^2 ORBITAL

We will see here that the next sp^2 orbital is canted relative to the first one we drew. Actually, as shown in some texts, they are 120° apart, as is the last one. Thus the trigonal structure of sp^2 central atom bonding is established.

Figure 4 shows the $\psi_{sp^2}(x, y, 0)$ versus x and y , while Figures 5 and 6 show the contour map and contour surface, respectively of this canted orbital.

IX. MAPLE

To help in this learning, perhaps the following code will be found useful.

```
> #sp2-hybrid-plot
> restart;
> with(plots);
> fs := exp(-r/2);
> psi_2s := (2-r)*fs;
> cart_psi_2p_x := x*fs;
> cart_psi_2p_y := y*fs;
> cart_psi_2p_z := z*fs;
> psi_2p_x := r*sin(theta)*cos(phi)*fs;
> psi_2p_y := r*sin(theta)*sin(phi)*fs;
> psi_2p_z := r*cos(theta)*fs;
> t11 := int(r^2*sin(theta)*psi_2p_x^2, phi=0..2*Pi):
> t21 := int(t11, theta=0..Pi):
> t31 := int(t21, r=0..infinity):
> N_2px := sqrt(t31);
> t12 := int(r^2*sin(theta)*psi_2s^2, phi=0..2*Pi):
> t22 := int(t12, theta=0..Pi):
> t32 := int(t22, r=0..infinity):
> N_2s := sqrt(t32);
> print ('the normalization constants are the
same, so we can ignore
> them');
```

Warning, the name changecoords has been redefined

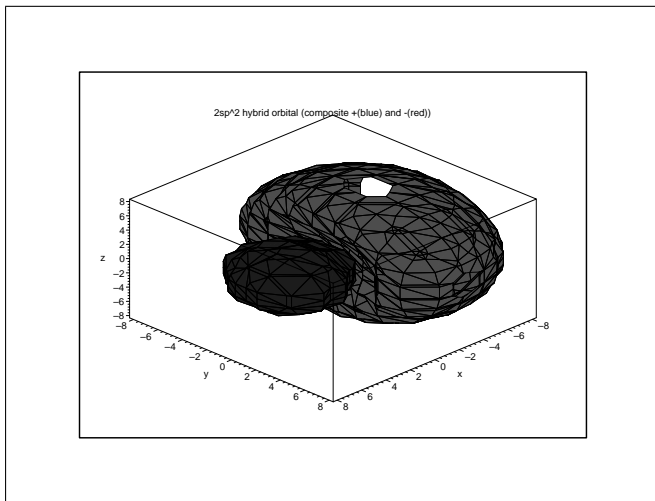


FIG. 3: $\psi = \text{constant}$ contour 3D plot. This is a composite, with the positive and negative lobes colored differently.

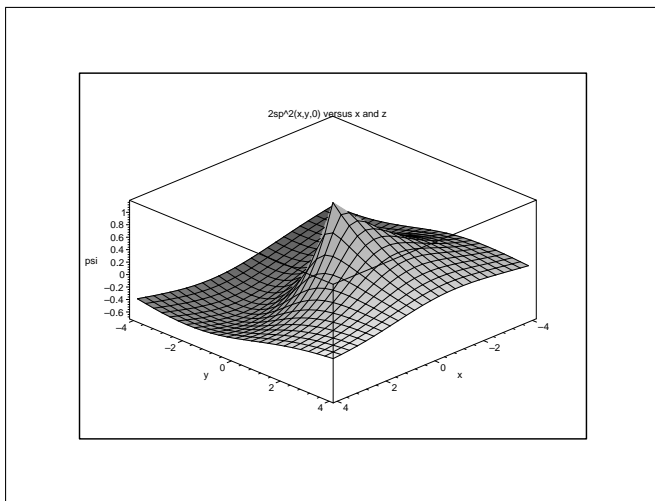


FIG. 4: Similar to the first sp^2 orbital, but pointing elsewhere. Again, notice the captioning error.

[*animate, animate3d, animatecurve, arrow, changecoords, complexplot, complexplot3d, conformal, conformal3d, contourplot, contourplot3d, coordplot, coordplot3d, cylinderplot, densityplot, display, display3d, fieldplot, fieldplot3d, gradplot, gradplot3d, graphplot3d, implicitplot, implicitplot3d, inequal, interactive, listcontplot, listcontplot3d, listdensityplot, listplot, listplot3d, loglogplot, logplot, matrixplot, odeplot, pareto, plotcompare, pointplot, pointplot3d, polarplot, polygonplot, polygonplot3d, polyhedra_supported, polyhedraplot, replot, rootlocus, semilogplot, setoptions, setoptions3d, spacecurve, sparsematrixplot, sphereplot, surfdata, textplot, textplot3d, tubeplot*]

$$f_s := e^{-\frac{r}{2}}$$

$$\psi_{2s} := (2 - r) e^{-\frac{r}{2}}$$

$$\text{cart_}\psi_{2p_x} := x e^{-\frac{r}{2}}$$

$$\text{cart_}\psi_{2p_y} := y e^{-\frac{r}{2}}$$

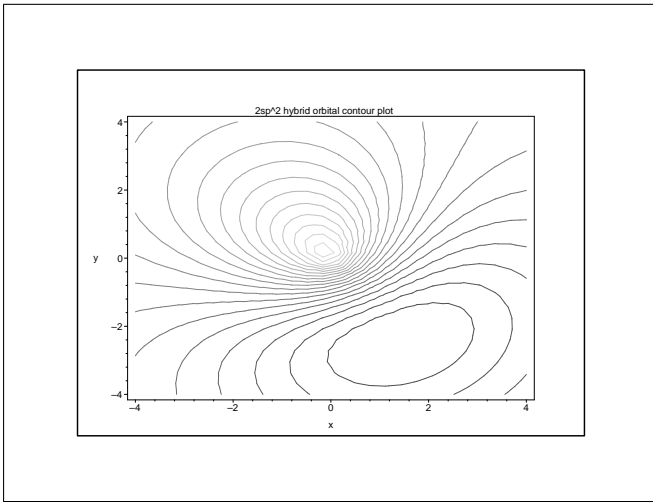


FIG. 5: The contour map of the second sp^2 orbital.

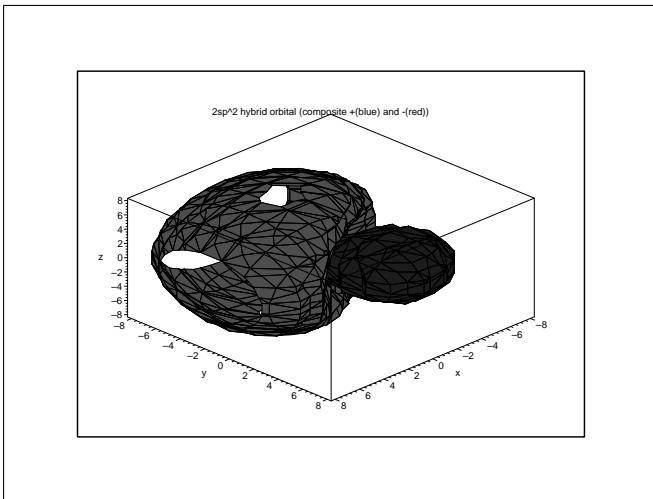


FIG. 6: The pseudo 3D implicitplot03D surface of $\psi(x, y, z)$ versus x , y , and z . This is a composite of the two lobes, one positive, one negative.

$$\begin{aligned}
 cart_psi_2p_z &:= z e^{-\frac{r}{2}} \\
 psi_2p_x &:= r \sin(\theta) \cos(\phi) e^{-\frac{r}{2}} \\
 psi_2p_y &:= r \sin(\theta) \sin(\phi) e^{-\frac{r}{2}} \\
 psi_2p_z &:= r \cos(\theta) e^{-\frac{r}{2}} \\
 N_2px &:= 4 \sqrt{2} \sqrt{\pi} \\
 N_2s &:= 4 \sqrt{2} \sqrt{\pi}
 \end{aligned}$$

the normalization constants are the same, so we can ignore them

```

> #note, un-normalized orbitals in use!
> r := sqrt(x^2+y^2+z^2):
> t1 := ((1/sqrt(3))*psi_2s+(sqrt(2/3))*cart_psi_2p_x);#page 372
> Karplus & Porter
> lim := 4;
> plot3d(subs(z=0,t1),x=-lim..lim,y=-lim..lim,axes=BOXED,labels=['x','y',
> 'psi'],title='2sp^2(x,y,0) versus x and z');
> contourplot(subs(z=0,t1),x=-lim..lim,y=-lim..lim,axes=BOXED,labels=['x',
> 'y'],title='2sp^2 hybrid orbital contour plot ',contours = 20);
> lim := 8;
> f1 :=
> implicitplot3d(t1=0.08,x=-lim..lim,y=-lim..lim,z=-lim..lim,axes=BOXED,
> labels=['x','y','z'],color=blue):
> f2 :=
> implicitplot3d(t1=-0.08,x=-lim..lim,y=-lim..lim,z=-lim..lim,axes=BOXED
> ,labels=['x','y','z'],title='2sp^2 hybrid orbital (composite +(blue)
> and -(red))',color=red):
> display(f1,f2);
> #=====
> t2 := ((1/sqrt(3))*psi_2s-(sqrt(1/6))*cart_psi_2p_x
> +(1/sqrt(2))*cart_psi_2p_y);#page 372 Karplus & Porter
> lim := 4;
> plot3d(subs(z=0,t2),x=-lim..lim,y=-lim..lim,axes=BOXED,labels=['x','y',
> 'psi'],title='2sp^2(x,y,0) versus x and z');
> contourplot(subs(z=0,t2),x=-lim..lim,y=-lim..lim,axes=BOXED,labels=['x',
> 'y'],title='2sp^2 hybrid orbital contour plot ',contours = 20);
> lim := 8;
> f1 :=
> implicitplot3d(t2=0.08,x=-lim..lim,y=-lim..lim,z=-lim..lim,axes=BOXED,
> labels=['x','y','z'],color=blue):
> f2 :=
> implicitplot3d(t2=-0.08,x=-lim..lim,y=-lim..lim,z=-lim..lim,axes=BOXED
> ,labels=['x','y','z'],title='2sp^2 hybrid orbital (composite +(blue)
> and -(red))',color=red):
> display(f1,f2);

```

$$t1 := \frac{1}{3} \sqrt{3} (2 - \sqrt{x^2 + y^2 + z^2}) e^{-\frac{\sqrt{x^2 + y^2 + z^2}}{2}} + \frac{1}{3} \sqrt{6} x e^{-\frac{\sqrt{x^2 + y^2 + z^2}}{2}}$$

$$\text{lim} := 4$$

$$\text{lim} := 8$$

$$t2 := \frac{1}{3} \sqrt{3} (2 - \sqrt{\%1}) e^{-\frac{\sqrt{\%1}}{2}} - \frac{1}{6} \sqrt{6} x e^{-\frac{\sqrt{\%1}}{2}} + \frac{1}{2} \sqrt{2} y e^{-\frac{\sqrt{\%1}}{2}}$$

$$\%1 := x^2 + y^2 + z^2$$

$$\text{lim} := 4$$

$$\text{lim} := 8$$

[1] M. Karplus and R. N. Porter, "Atoms & Molecules", W. A. Benjamin, Inc., Phillipines, 1970.