How Good are the Hartree-Fock Nodes?

(for spin-up electrons on a sphere)

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Molecular Electronic Structure, Amasya, Turkey

3rd September 2014

Nodes, Nodal Pockets and Fixed-Node Approximation

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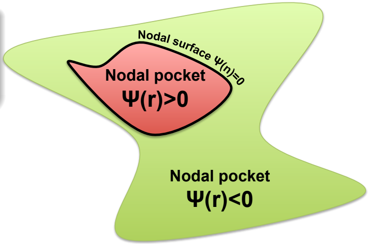
What's a node?

node = point in configuration space **n** for which $\Psi(\mathbf{n}) = 0$



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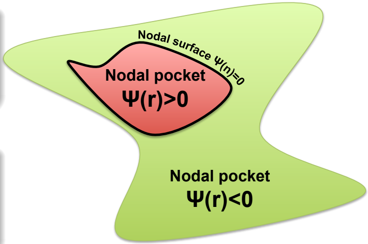

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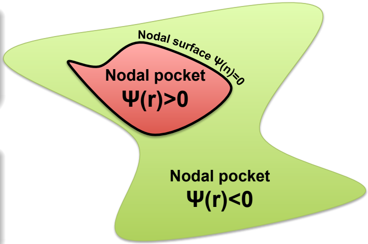

Why is it important to know the nodes?

- ☹ Vanilla **DMC** algorithm converges to bosonic ground state
- ☺ Nodes of the **trial** wave function has to be fixed: fixed-node (FN) approximation
- ☹ FN-DMC gives **exact** energy iff the nodes are **exact**
- ☺ FN **error** proportional to the square of the node displacement
- ☹ FN **error** very hard to estimate
- ☹ Nodes poorly understood due to high dimensionality of nodal **hypersurface**

Electrons on a Ring

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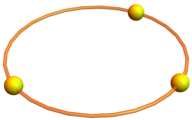

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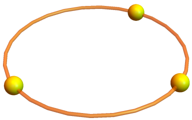

… when 2 electrons touch!

$$\Psi_{\text{HF}}^{\text{1D}} = \begin{vmatrix} e^{-i\,\phi_1} & 1 & e^{+i\,\phi_1} \\ e^{-i\,\phi_2} & 1 & e^{+i\,\phi_2} \\ e^{-i\,\phi_3} & 1 & e^{+i\,\phi_3} \end{vmatrix} \propto r_{12}\, r_{13}\, r_{23}$$

Mitas, PRL 96 (2006) 240402
Loos & Gill, PRL 108 (2012) 083002

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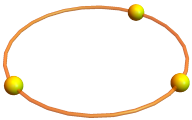

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Reduced correlation energy (in millihartree) for n electrons on a ring

		Seitz radius r_s										
n	η	0	0.1	0.2	0.5	1	2	5	10	20	50	100
2	3/4	13.212	12.985	12.766	12.152	11.250	9.802	7.111	4.938	3.122	1.533	0.848
3	8/9	18.484	18.107	17.747	16.755	15.346	13.179	9.369	6.427	4.030	1.965	1.083
4	15/16	21.174	20.698	20.249	19.027	17.324	14.762	10.390	7.085	4.425	2.150	1.184
5	24/25	22.756	22.213	21.66	20.33	18.439	15.644	10.946	7.439	4.636	2.248	1.237
6	35/36	23.775	23.184	22.63	21.14	19.137	16.192	11.285	7.653	4.762	2.307	1.268
7	48/49	24.476	23.850	23.24	21.70	19.607	16.554	11.509	7.795	4.844	2.345	1.289
8	63/64	24.981	24.328	23.69	22.11	19.940	16.808	11.664	7.890	4.901	2.370	1.302
9	80/81	25.360	24.686	24.04	22.39	20.186	16.995	11.777	7.960	4.941	2.389	1.312
10	99/100	25.651	24.960	24.25	22.62	20.373	17.134	11.857	8.013	4.973	2.404	1.320
∞	1	27.416	26.597	25.91	23.962	21.444	17.922	12.318	8.292	5.133	2.476	1.358

Loos & Gill, JCP 138 (2013) 164124; Loos, Ball & Gill, ibid 140 (2014) 18A524

Why on a Sphere?

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Electrons on a sphere are cool!

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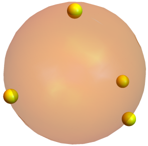

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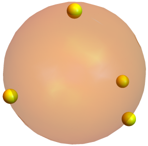

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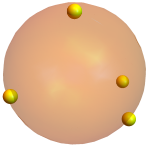

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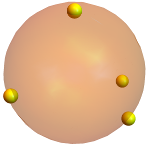

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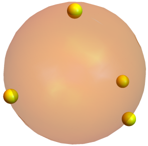

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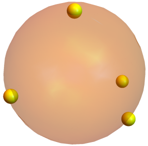
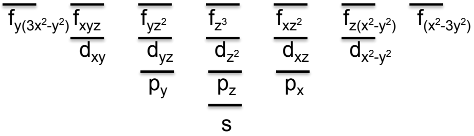


Spherical coordinates

$$x = \cos\phi \sin\theta$$
$$y = \sin\phi \sin\theta$$
$$z = \cos\theta$$

HF orbitals on a sphere: $s, p, d, f, g, h, i, j, \ldots$



Loos & Gill, PRA 79 (2009) 062517; PRL 103 (2009) 123008; Mol. Phys. 108 (2010) 2527.

Two Electrons on a Sphere

$\mathbf{z} = (0,0,1)$ is the unit vector of the z axis, $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$, $\mathbf{r}_{ij}^{+} = \mathbf{r}_i + \mathbf{r}_j$ and $\mathbf{r}_{ij}^{\times} = \mathbf{r}_i \times \mathbf{r}_j$

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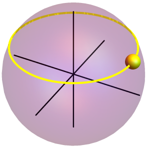
Two Electrons on a Sphere

***sp* state:** $^3P^o$

$$\Psi_{\text{HF}} = \begin{vmatrix} 1 & z_1 \\ 1 & z_2 \end{vmatrix} = \mathbf{z} \cdot \mathbf{r}_{12}$$



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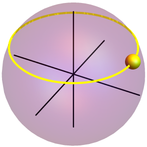

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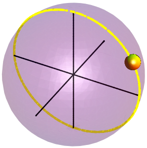

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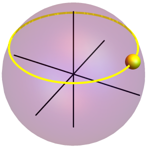

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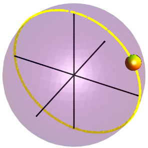
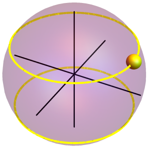


sd state: $^3D^e$

$$\Psi_{\text{HF}} = \begin{vmatrix} 1 & x_1\, y_1 \\ 1 & x_2\, y_2 \end{vmatrix} = (\mathbf{z} \cdot \mathbf{r}_{12}^{+})(\mathbf{z} \cdot \mathbf{r}_{12})$$



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Are the HF nodes of the p^3 state exact?

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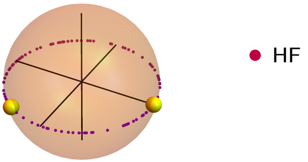
$|\Psi_{HF}|$ = volume of parallelepiped

HF nodes vs FCI nodes



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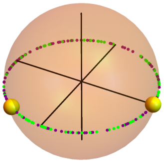

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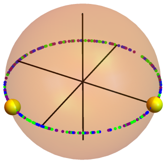

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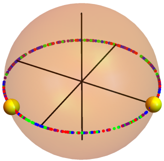

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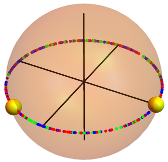

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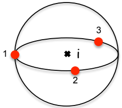
Proof: great circles are nodes!



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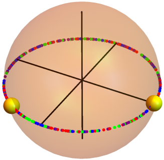

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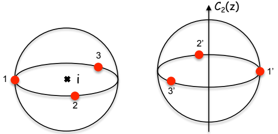

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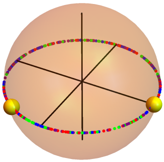

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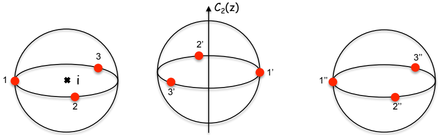

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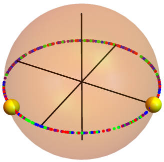

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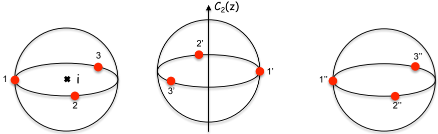

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Connection 2D → 1D

if $\theta_1 = \theta_2 = \theta_3 \neq 0$ or $\pi/2$

$$\Rightarrow \Psi_{\text{HF}} = \begin{vmatrix} 1 & y_1 & z_1 \\ 1 & y_2 & z_2 \\ 1 & y_3 & z_3 \end{vmatrix} = \Psi_{\text{HF}}^{\text{1D}}$$

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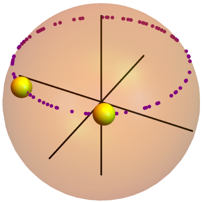

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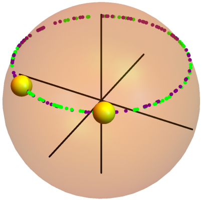

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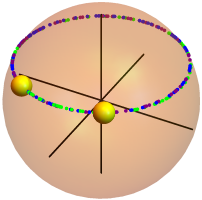

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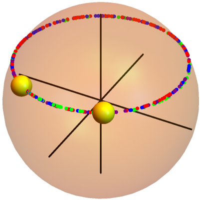

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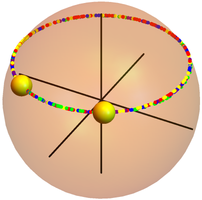

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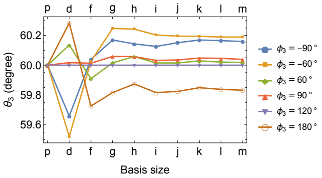

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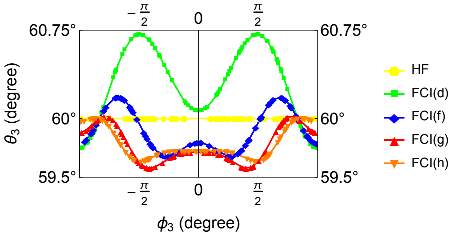

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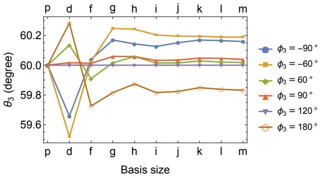

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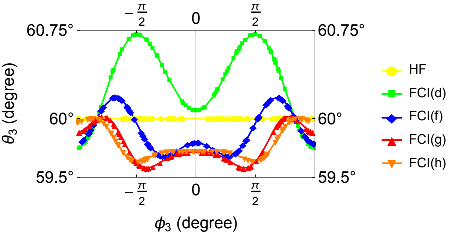

The HF nodes of the sp^2 state are **not** exact!

... but not too bad!

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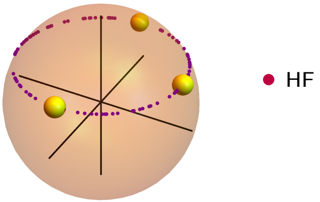

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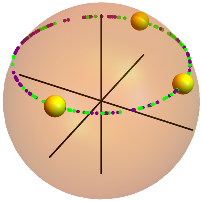

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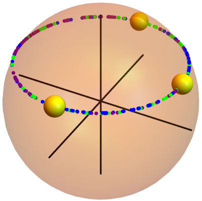

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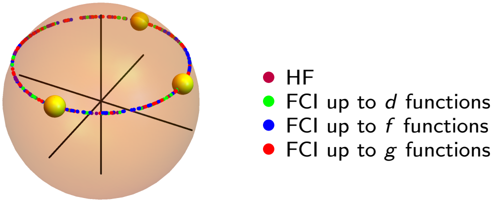

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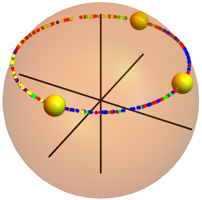

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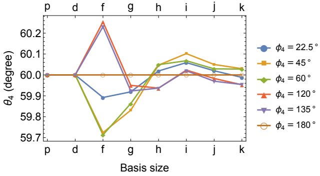

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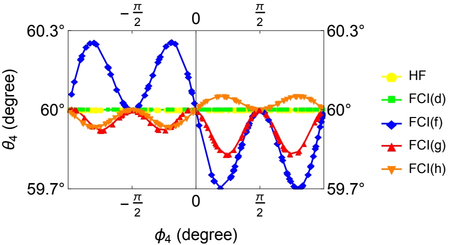

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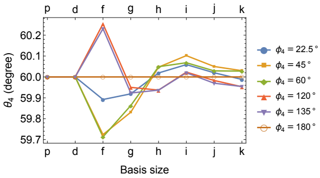

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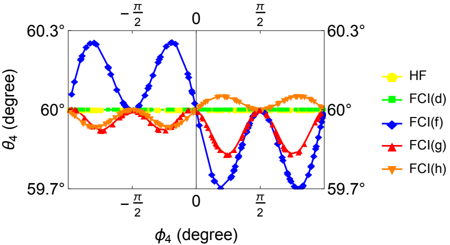

The HF nodes of the sp^3 state **could be** exact!

... if not, they're really good!

Concluding remarks

For same-spin electrons on a sphere,

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- It can be generalized to **more electrons** and **higher dimensions**

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Dario Bressanini

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Australian Research Council

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