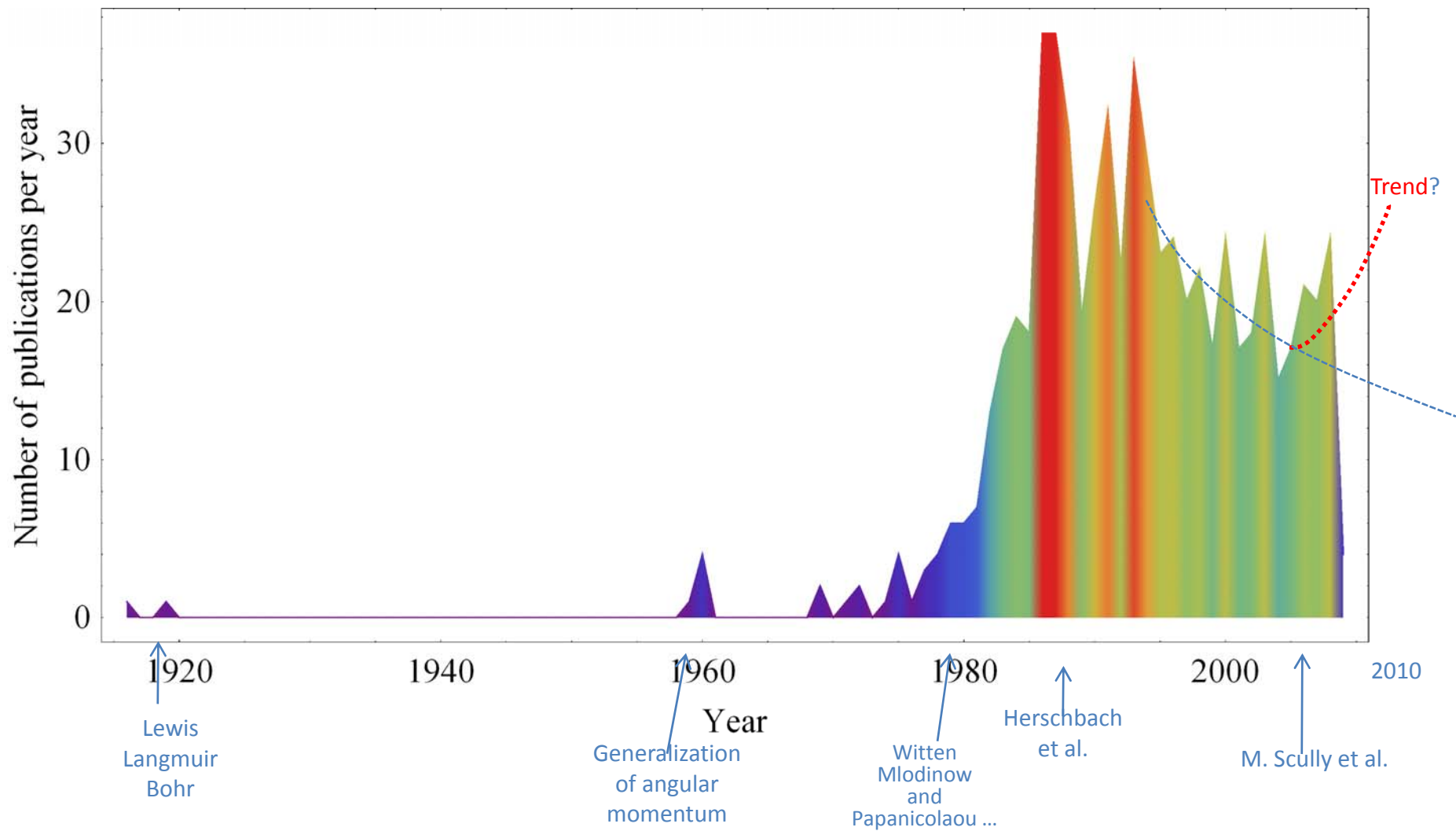


Generalizations of Bohr Model and *D*-scaling Method

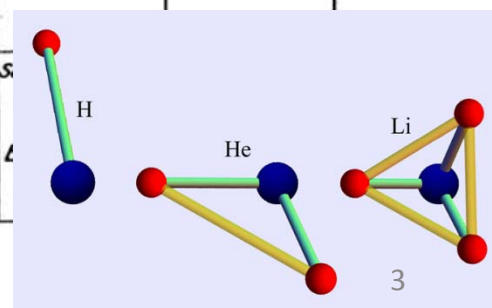
Alexey Sergeev

1. Hydrogen atom
2. Helium
3. H₂ molecule
4. Many-electron atoms (with new results)



<i>E=0</i>	1	2	3	4	5	6	7	8	9	10
<i>He</i> 2	<i>Li</i> 3	<i>Be</i> 4	<i>B</i> 5	<i>C</i> 6	<i>N</i> 7	<i>O</i> 8	<i>F</i> 9			
<i>Ne</i> 10	<i>Na</i> 11	<i>Mg</i> 12	<i>Al</i> 13	<i>Si</i> 14	<i>P</i> 15	<i>S</i> 16	<i>Cl</i> 17			
<i>A</i> 18	<i>K</i> 19	<i>Ca</i> 20	<i>Sc</i> 21	<i>Ti</i> 22	<i>V</i> 23	<i>Cr</i> 24	<i>Mn</i> 25	<i>Fe</i> 26	<i>Co</i> 27	<i>Ni</i> 28
<i>Niβ</i> 29	<i>Cu</i> 30	<i>Zn</i> 31	<i>Ga</i> 32	<i>Ge</i> 33	<i>As</i> 34	<i>Se</i> 35	<i>Br</i> 36			
<i>Kr</i> 37	<i>Rb</i> 38	<i>Sr</i> 39	<i>Y</i> 40	<i>Zr</i> 41	<i>Cb</i> 42	<i>Mo</i> 43	<i>Ru</i> 44	<i>Rh</i> 45	<i>Pd</i> 46	
<i>Pdβ</i> 47	<i>Ag</i> 48	<i>Cd</i> 49	<i>In</i> 50	<i>Sn</i> 51	<i>Sb</i> 52	<i>Te</i> 53	<i>I</i> 54			
<i>Xe</i> 55	<i>Cs</i> 56	<i>Ba</i> 57	<i>La</i> 58	<i>Ce</i> 59	<i>Pr</i> 60	<i>Nd</i> 61	<i>S</i> 62			

CHART I.—Illustrating the Lewis-Langmuir Theory of Atomic Structure.



Year 1959

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Year 1960

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Invariance of the correlation energy at high density and large dimension in two-electron systems

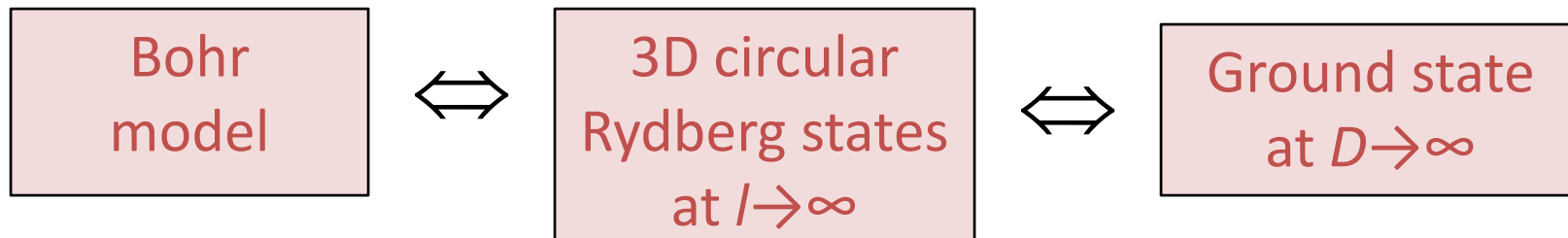
Pierre-François Loos* and Peter M. W. Gill†

*Research School of Chemistry, Australian National University,
Canberra, Australian Capital Territory, 0200, Australia*

(Dated: July 19, 2010)

We prove that, in the large-dimension limit, the high-density correlation energy E_c of two opposite-spin electrons confined in a D -dimensional space and interacting *via* a Coulomb potential is given by $E_c \sim -1/(8D^2)$ for any radial confining potential $V(r)$. This result explains the observed similarity of E_c in a variety of two-electron systems in three-dimensional space.

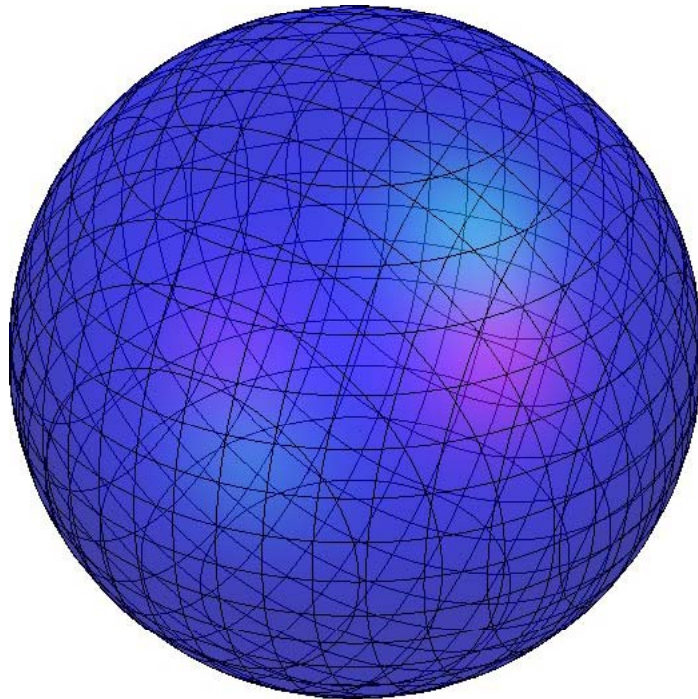
Hydrogen atom, Bohr model and large D limit



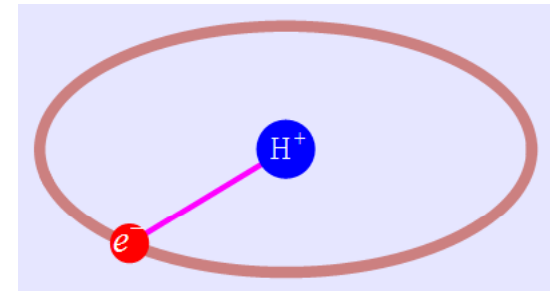
$$\Psi_{nlm} = r^l e^{-r/n} L_{n-l-1}^{2l+1}(2r/n) Y_l^m(\theta, \varphi)$$

Ground state

$$\Psi_{100} = e^{-r}$$

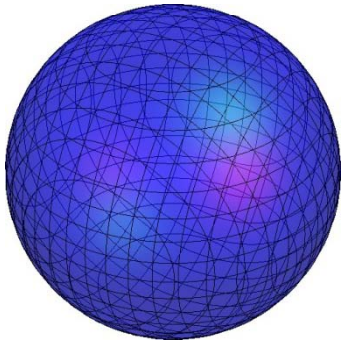


Bohr model

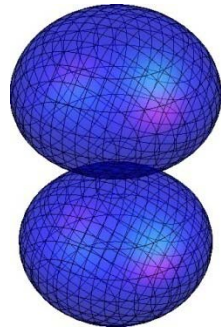


$n = 4$ states

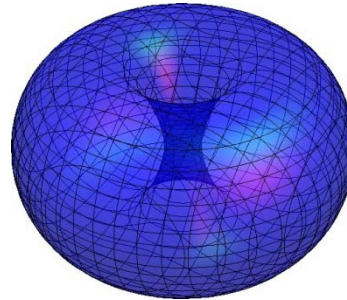
Ψ_{400}



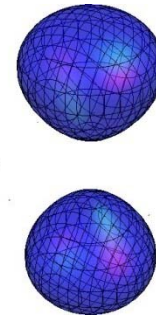
Ψ_{410}



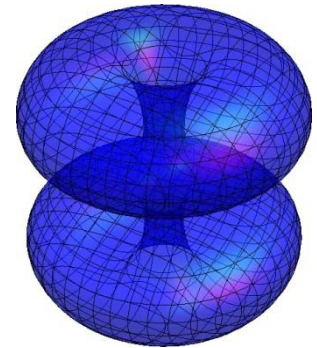
Ψ_{411}



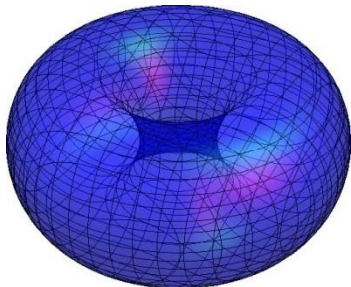
Ψ_{420}



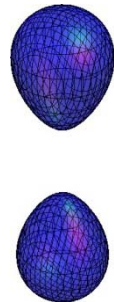
Ψ_{421}



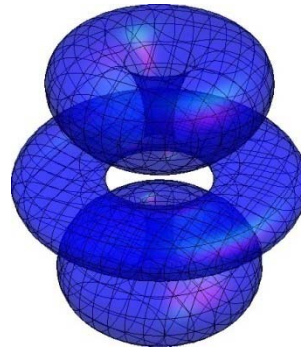
Ψ_{422}



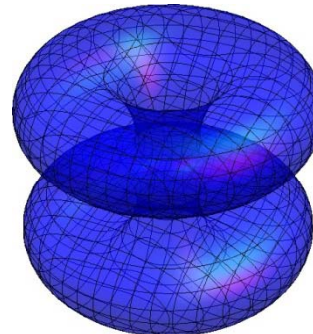
Ψ_{430}



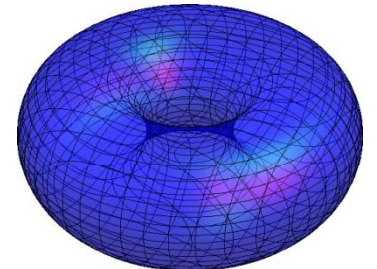
Ψ_{431}



Ψ_{432}



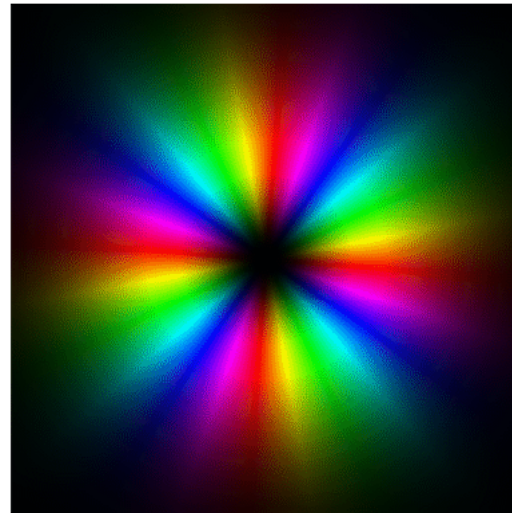
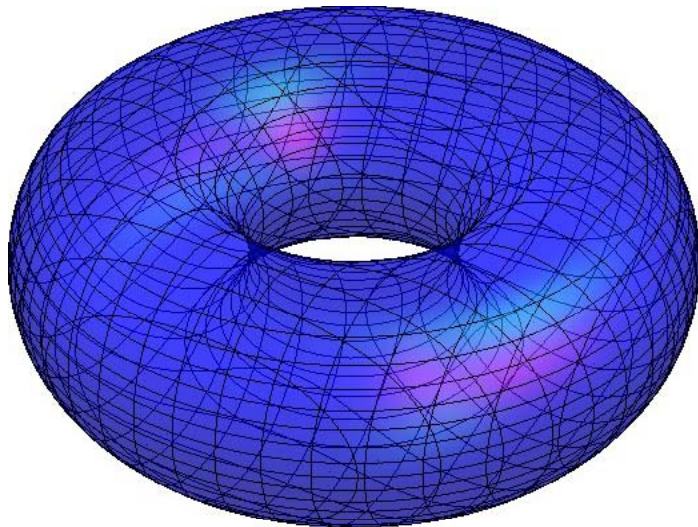
Ψ_{433}



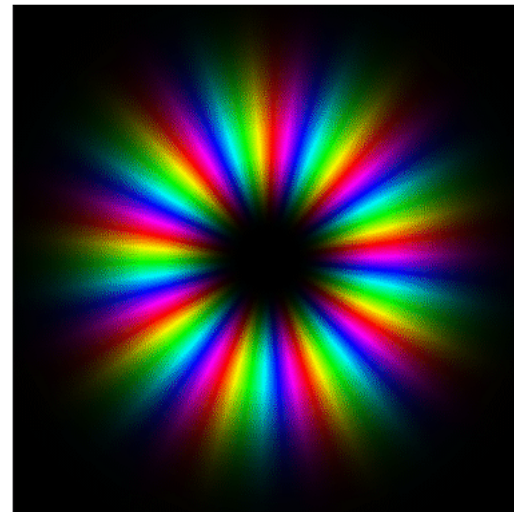
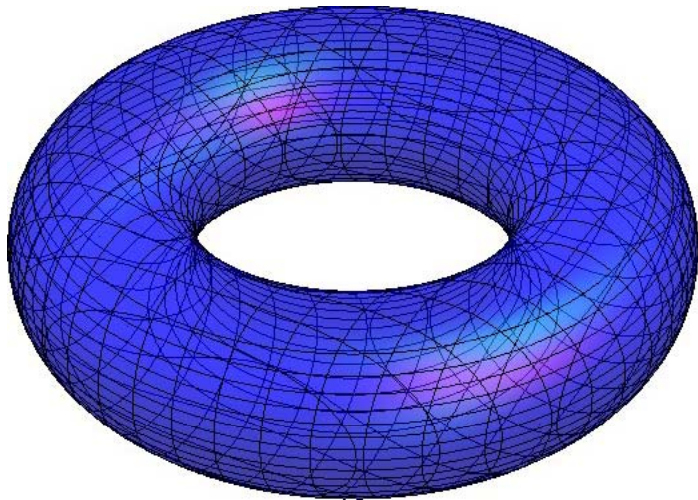
Circular Rydberg states $(n, n-1, n-1)$

$$l = n - 1, \quad m = l$$

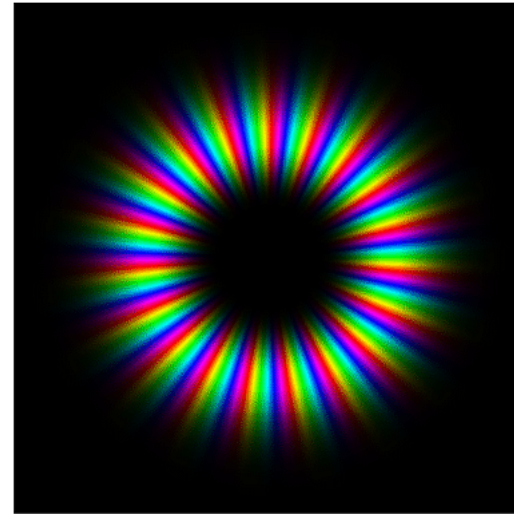
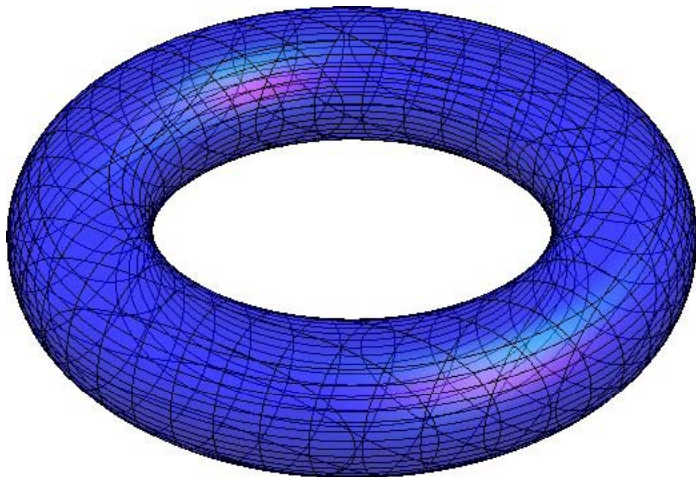
$$n = 5$$



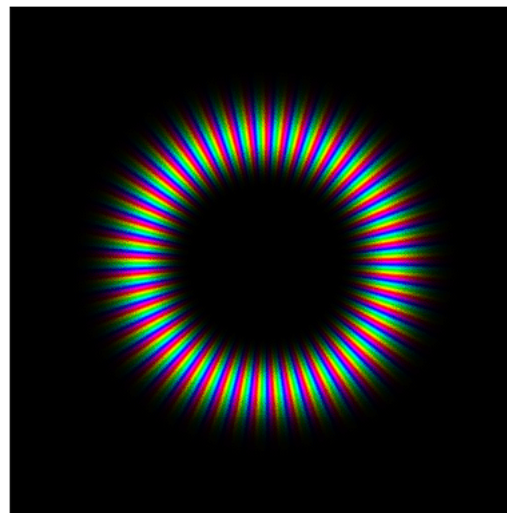
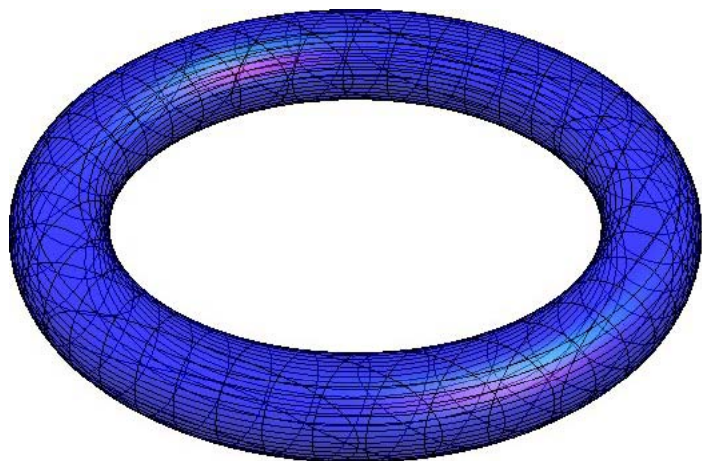
$$\Psi_{10,9,9} \quad (n = 10)$$



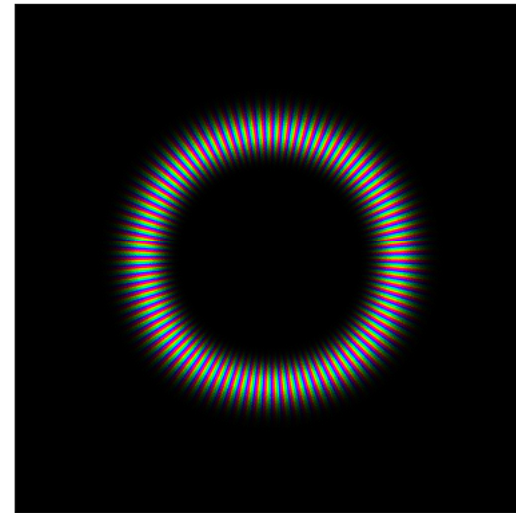
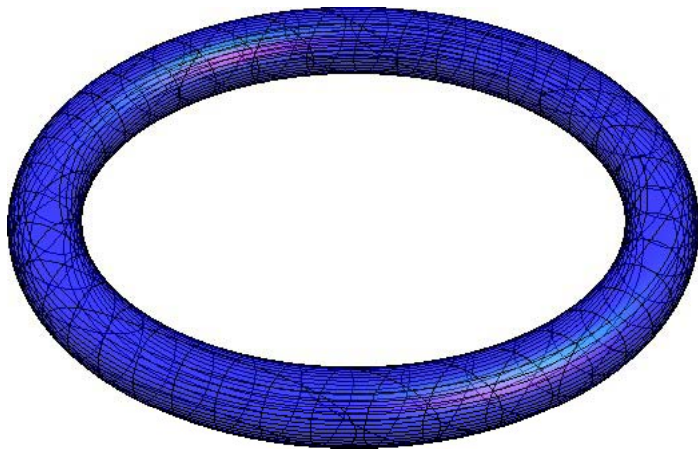
$$\Psi_{20,19,19} \quad (n = 20)$$



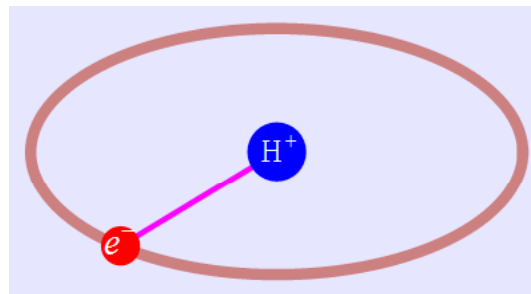
$$\Psi_{50,49,49} \quad (n = 50)$$



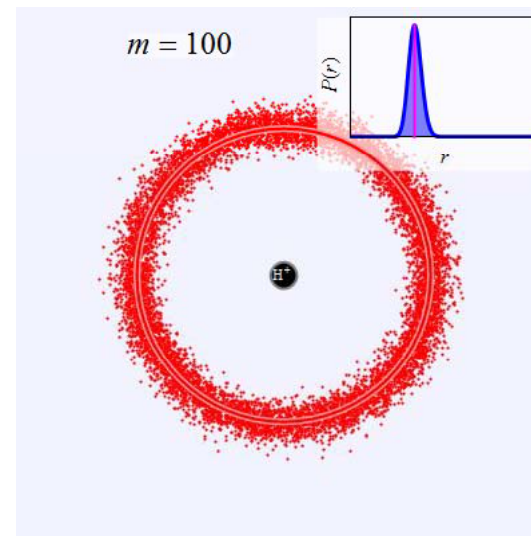
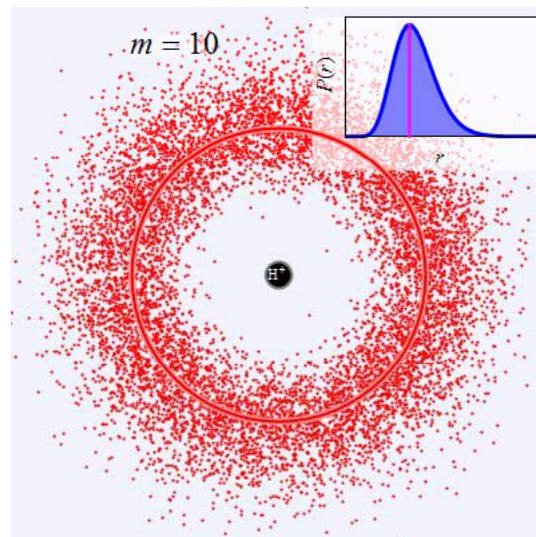
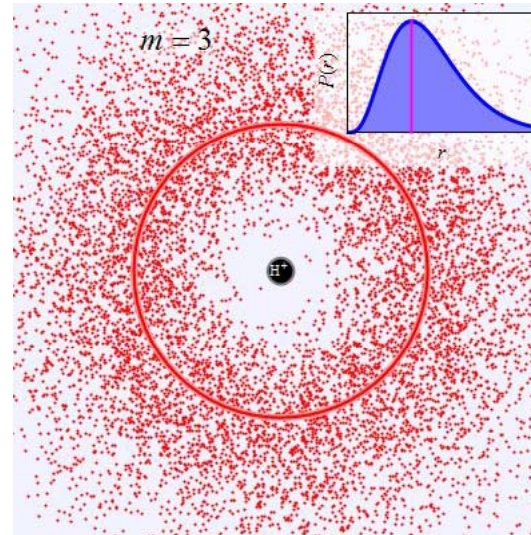
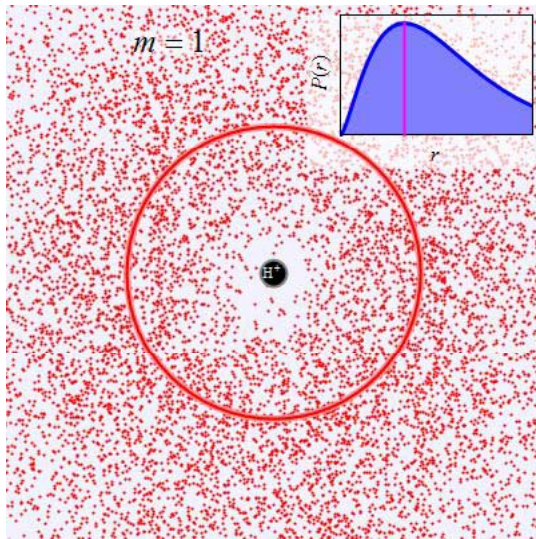
$$\Psi_{100,99,99} \quad (n = 100)$$



$$n \rightarrow \infty$$



$$r^2 |\Psi|^2 \rightarrow \delta(r - r_0)$$



Interdimensional degeneracy

$m=l$ state: $\Psi(\vec{r}) = (x + iy)^l \chi(r)$

$$\left[-\frac{1}{2r^{2(l+1)}} \frac{d}{dr} r^{2(l+1)} \frac{d}{dr} + V(r) - E \right] \chi(r) = 0$$

$l=0$ state in D dimensions: $\Psi^{(D)}(\vec{r}) = R(r)$

$$\left[-\frac{1}{2r^{D-1}} \frac{d}{dr} r^{D-1} \frac{d}{dr} + V(r) - E \right] R(r) = 0$$

$m=l$ state ($D=3$)



$l=0$ state ($D=3+2l$)

Two-electron atoms

$l=0$ state in D dimensions:

$$\Psi^{(D)}(\vec{r}_1, \vec{r}_2) = \psi(r_1, r_2, \theta)$$

$$\left\{ -\frac{1}{2} \left[\frac{1}{r_1^{D-1}} \frac{d}{dr_1} r_1^{D-1} \frac{d}{dr_1} + \frac{1}{r_2^{D-1}} \frac{d}{dr_2} r_2^{D-1} \frac{d}{dr_2} + \right. \right. \\ \left. \left. + \left(\frac{1}{r_1^2} + \frac{1}{r_2^2} \right) \frac{1}{\sin^{D-2} \theta} \frac{\partial}{\partial \theta} \sin^{D-2} \theta \frac{\partial}{\partial \theta} \right] + V(r_1, r_2, \theta) - E \right\} \psi(r_1, r_2, \theta) = 0$$

Circular states of helium in four dimensions

$$\Psi(\vec{r}_1, \vec{r}_2) = (x_1 + iy_1)^l (z_2 + iw_2)^l \chi(r_1, r_2, \theta)$$

$$L_{ij} = q_{1i}p_{1j} - q_{1j}p_{1i} + q_{2i}p_{2j} - q_{2j}p_{2i}$$

$$\mathbf{L} = \begin{pmatrix} 0 & l & 0 & 0 \\ -l & 0 & 0 & 0 \\ 0 & 0 & 0 & l \\ 0 & 0 & -l & 0 \end{pmatrix}$$

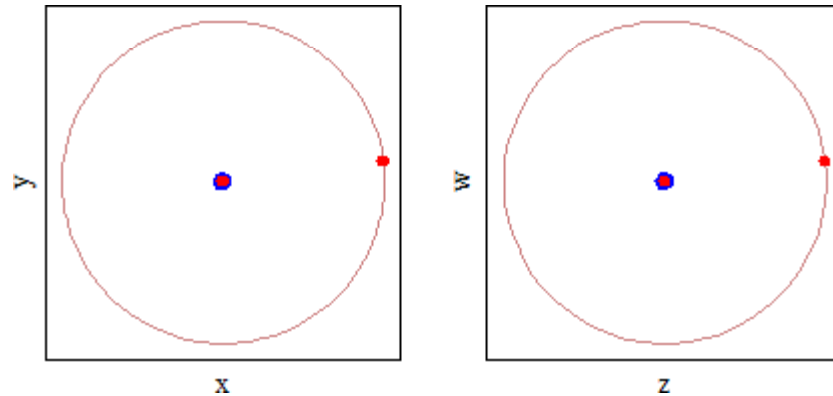
Interdimensional degeneracy

$$\left(\begin{array}{c} \text{Equation for} \\ \text{the function } \chi (D = 4) \end{array} \right) \Leftrightarrow \left(\begin{array}{c} \text{Equation for the function } R \\ \text{in which } D \rightarrow 4 + 2l \end{array} \right)$$

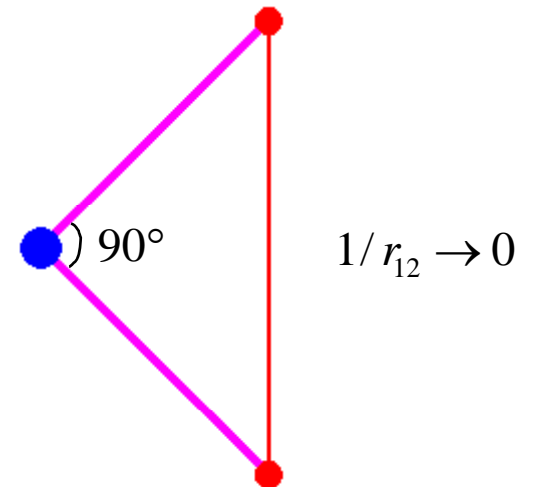
$$\boxed{l\text{-state } (D=4)} \Leftrightarrow \boxed{l=0 \text{ state } (D=4+2l)}$$

Bohr orbits for helium in four dimensions (x, y, z, w)

$$\begin{aligned}
 x_1(t) &= R \cos \omega t & x_2(t) &= 0 \\
 y_1(t) &= R \sin \omega t & y_2(t) &= 0 \\
 z_1(t) &= 0 & z_2(t) &= R \cos \omega t \\
 w_1(t) &= 0 & w_2(t) &= R \sin \omega t
 \end{aligned}$$



$$\begin{aligned}
 r_1(t) &= (x_1^2 + y_1^2 + z_1^2 + w_1^2)^{1/2} = R \\
 r_2(t) &= (x_2^2 + y_2^2 + z_2^2 + w_2^2)^{1/2} = R \\
 r_{12}(t) &= ((x_1 - x_2)^2 + (y_1 - y_2)^2 + (z_1 - z_2)^2 + (w_1 - w_2)^2)^{1/2} = \sqrt{2}R
 \end{aligned}$$



J. A. West et al., Classical limit states of the helium atom. Phys. Rev. A, 58, 186, 1998

The logical progression of the hydrogenic studies is to extend them to include planetary atoms with multiple valence electrons [2–6]. However, even for the simplest such atom, helium, this extension is nontrivial because the old quantum theory of Bohr was never successfully modified to include helium. Early in this century a considerable effort was made to develop a classical model for helium, but no stable planetary orbits were found [see Figs. 1(a) and 1(b)]. By 1920 Bohr had concluded that for stability, one must allow for “possibilities of more complicated motions,” [7] but before these possibilities could be explored, classical atomic physics was abandoned in the wake of wave mechanics and classical helium was put aside.

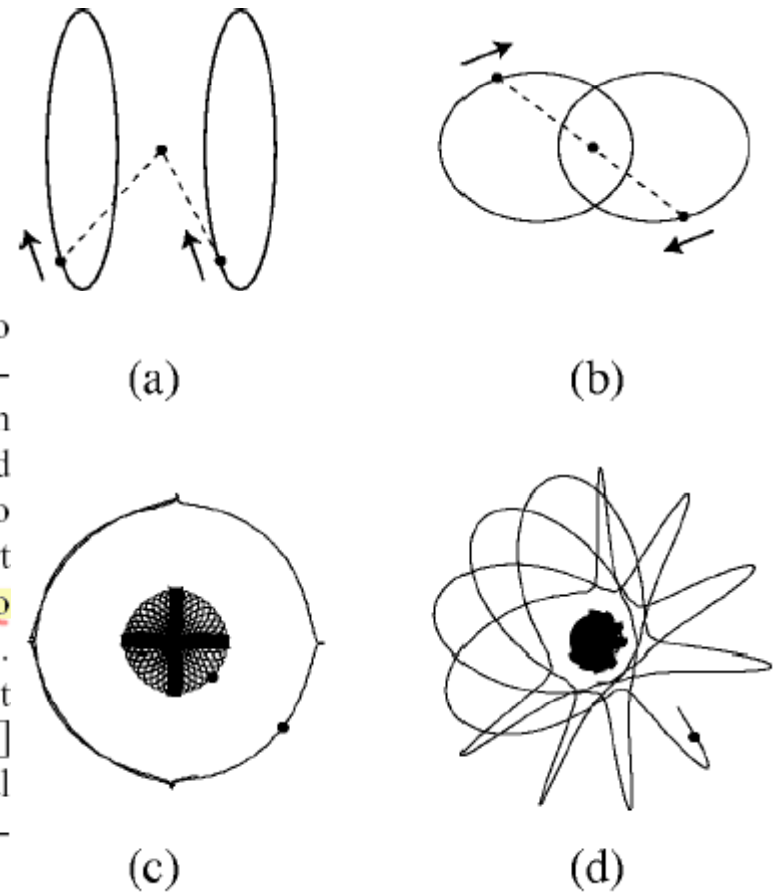
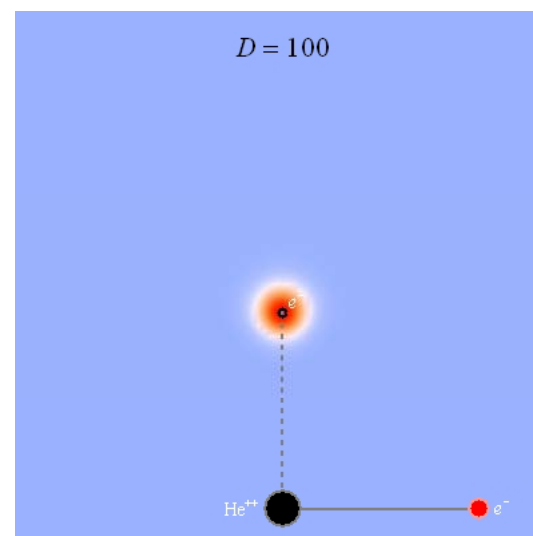
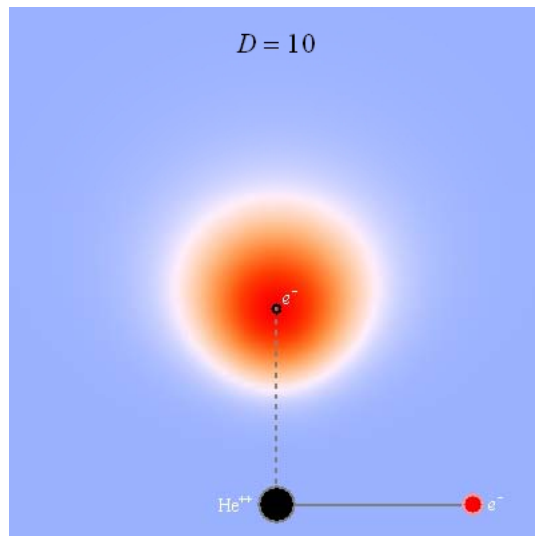
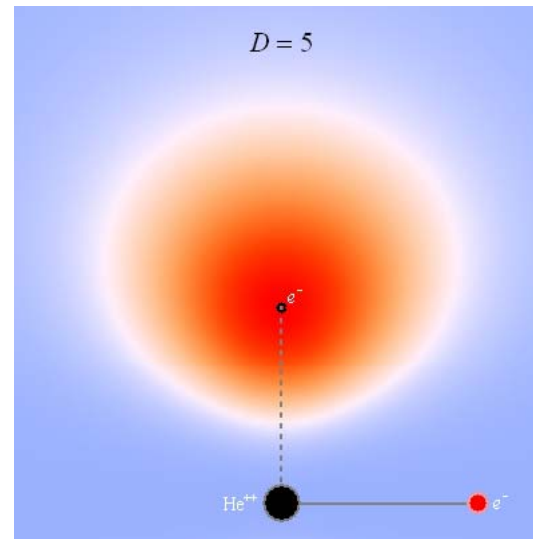
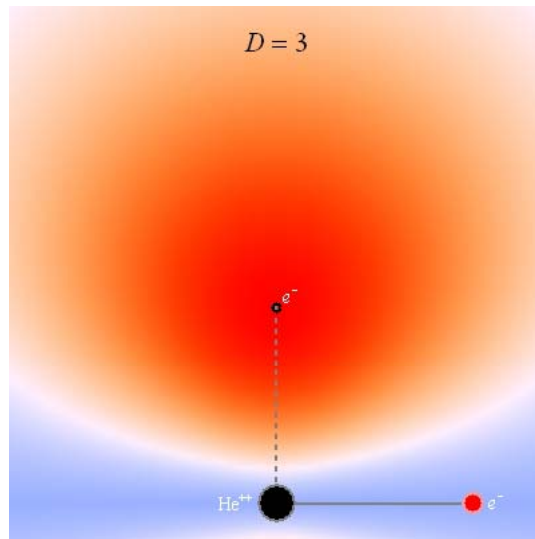


FIG. 1. A pictorial survey of some classical helium orbits. The two-electron trajectories shown in (a) and (b) are highly symmetric unstable orbits which were studied in an attempt to extend the Bohr model [3,7,8]. The orbits shown in (c) and (d) are stable orbits in which the dynamics of the individual electrons is quite dissimilar. In these orbits it is difficult to resolve the rapid motion of the inner electron.

Probability distribution of an electron in a helium atom in D dimensions

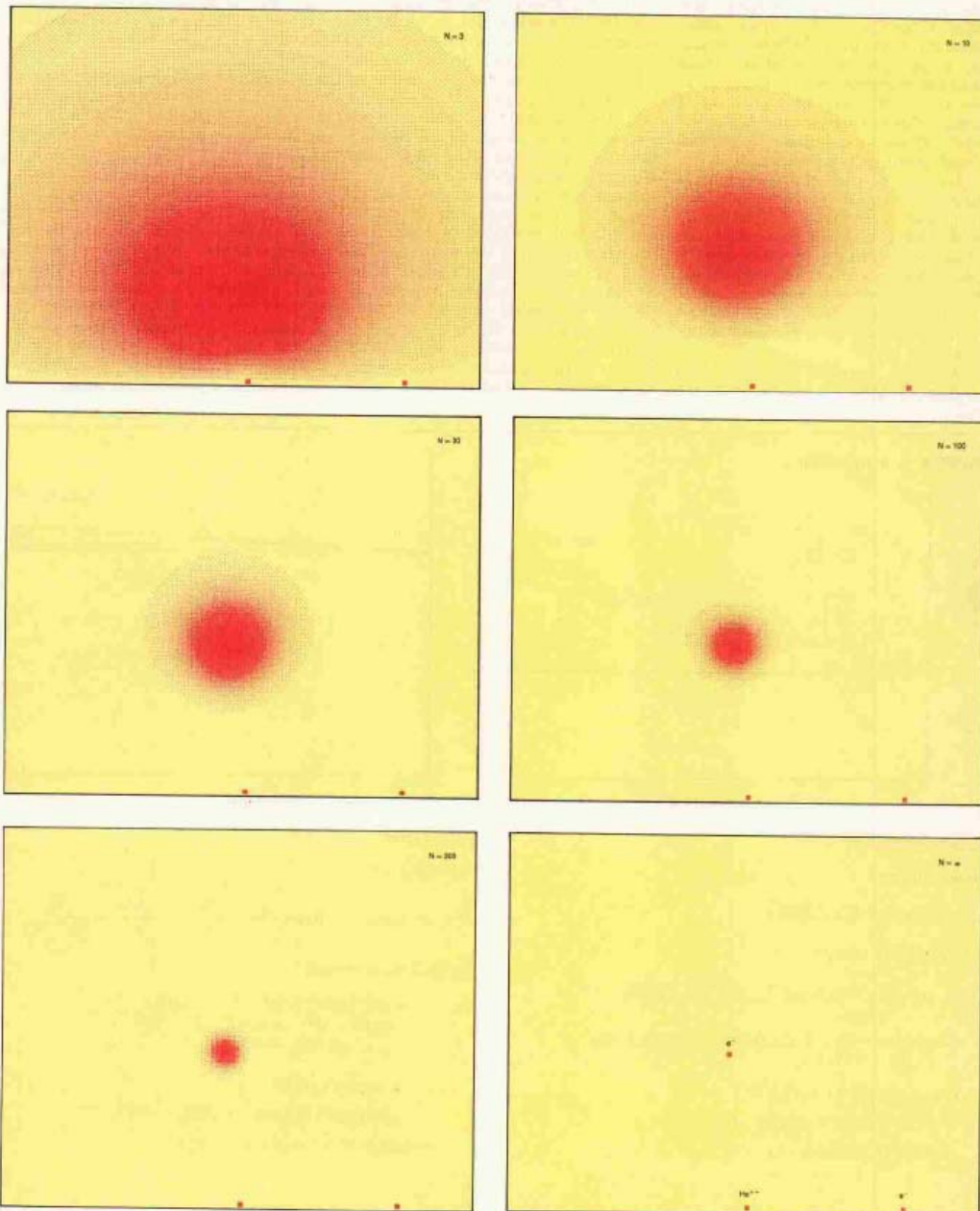


L. G. Yaffe,
Physics Today
(1982)

Large- N quantum mechanics and classical limits

Increasing the number of degrees of freedom surprisingly simplifies the analysis in many quantum theories, often making it possible to calculate physical observables.

Laurence G. Yaffe



Probability distribution of an electron in a helium atom in N dimensions, for six different values of N . The density of points is proportional to the probability of finding one electron at a given position relative to the nucleus and the other electron. The two small squares at the bottom of each of these computer-drawn pictures represent the helium atom's nucleus (left) and the fixed electron

(right). In each dimension, one electron is fixed at its root-mean-square distance from the nucleus. As the dimension increases, the probability distribution shrinks to a point. This is a consequence of the fact that the limit $N \rightarrow \infty$ is actually a novel type of classical limit. When N is infinite, one can compute the positions of the electrons directly by minimizing an appropriate classical Hamiltonian.

EFFECTIVE POTENTIAL FOR TWO-ELECTRON ATOMS

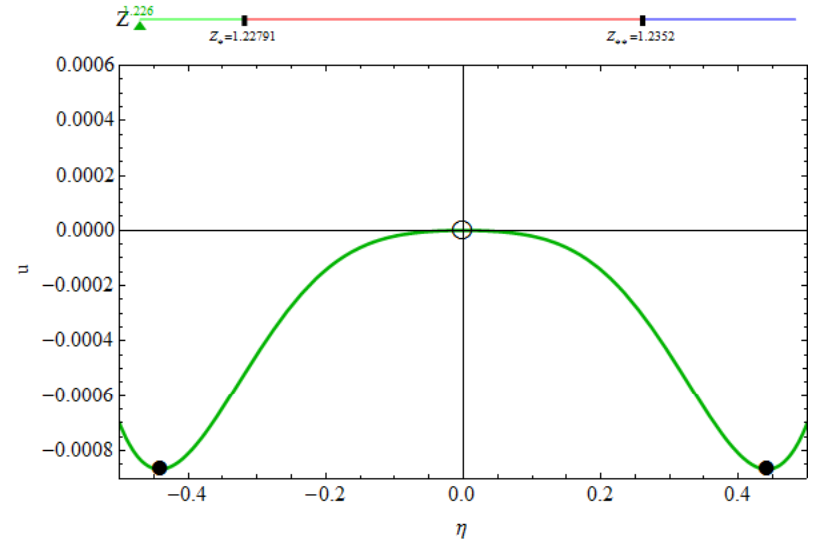
$$\tilde{U} = \frac{1}{2} \left(\frac{1}{\tilde{h}_1^2} + \frac{1}{\tilde{h}_2^2} \right) + \tilde{V},$$

$$\tilde{V} = -\frac{Z}{\tilde{r}_1} - \frac{Z}{\tilde{r}_2} + \frac{1}{\tilde{r}_{12}}, \quad \tilde{h}_1 = \tilde{r}_1 \sin \theta_{12}, \quad \tilde{h}_2 = \tilde{r}_2 \sin \theta_{12}.$$

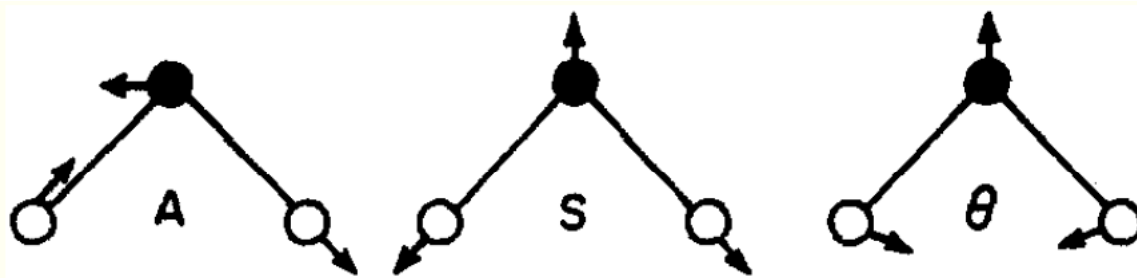
$$\tilde{E}_0 = \tilde{U} \left(\tilde{r}_1^{(0)}, \tilde{r}_2^{(0)}, \tilde{r}_{12}^{(0)} \right)$$

$$\eta = \frac{\tilde{r}_1 - \tilde{r}_2}{\tilde{r}_1 + \tilde{r}_2}, \quad -1 < \eta < 1$$

$$u(\eta) = \min \tilde{U} (\tilde{r}_1, \tilde{r}_2, \tilde{r}_{12})$$

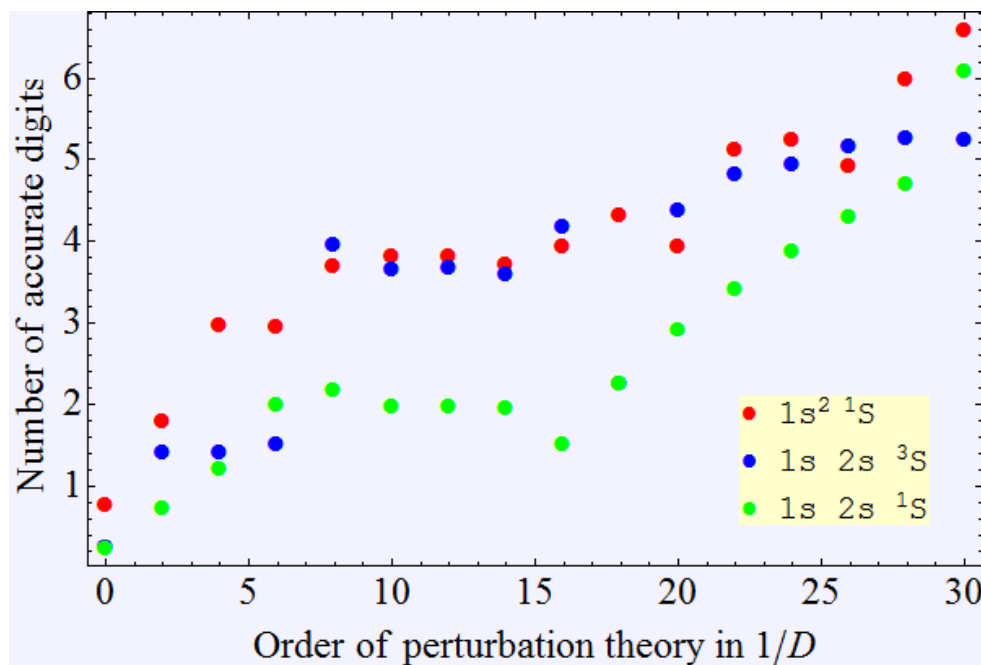
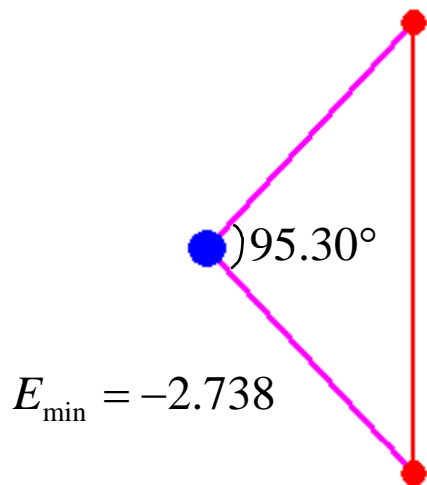


1/D-expansion

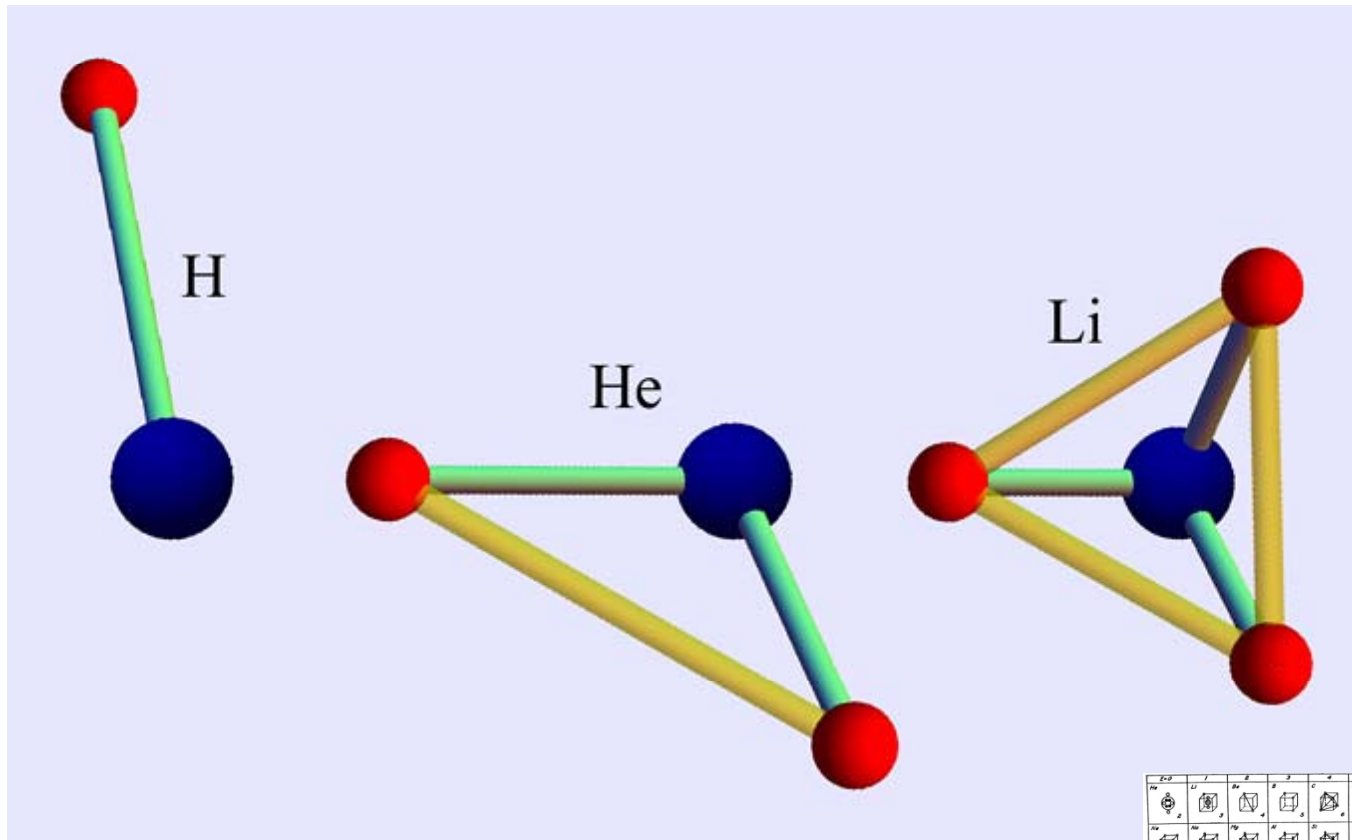


from the paper of Herschbach

Vibrations corresponding to antisymmetric stretch (A), symmetric stretch (S), and bend (θ) modes.



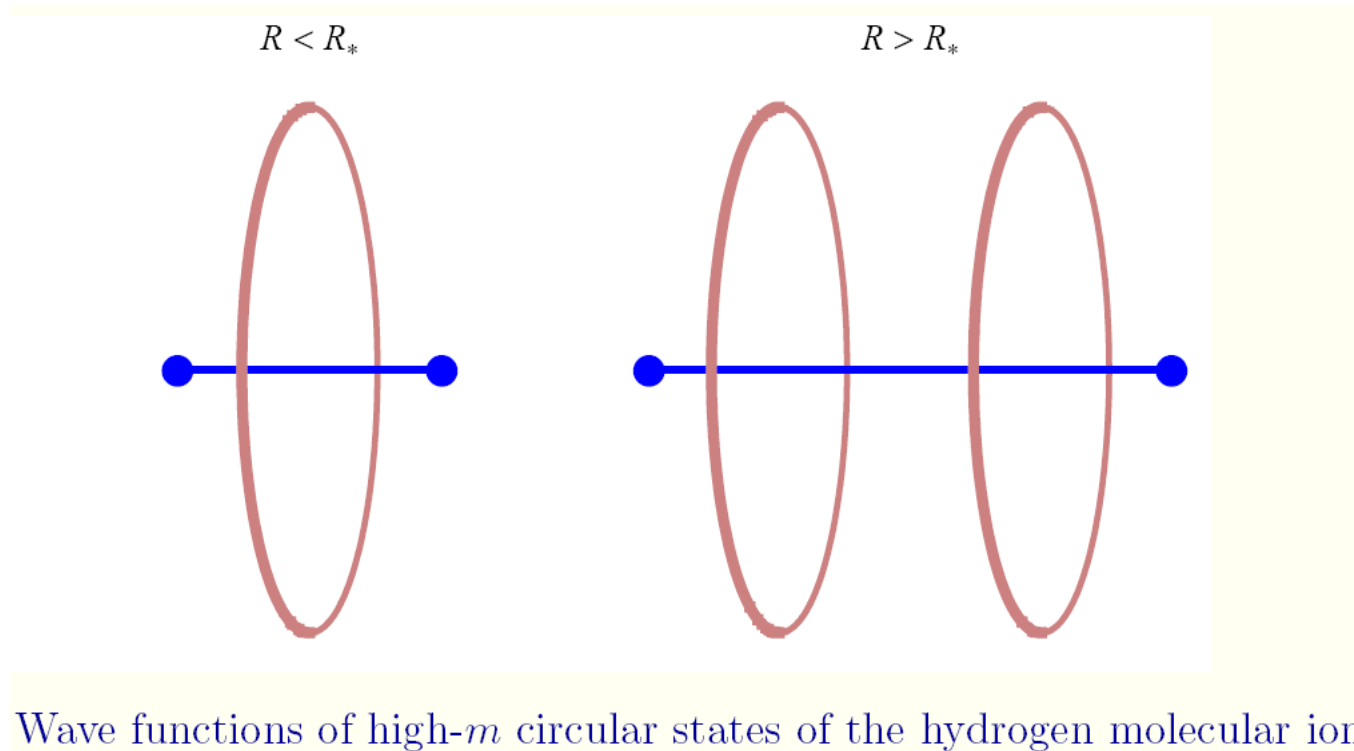
Atoms in the large D limit



$2\pi D$	1	2	3	4	5	6	7	8	9	10
$1s_1$										
$2s_1$										
$3s_1$										
$4s_1$										
$5s_1$										
$6s_1$										
$7s_1$										
$8s_1$										
$9s_1$										
$10s_1$										

28
 Chapter 1: Modeling the Shell-Like Theory of Atomic Structure

Hydrogen molecule

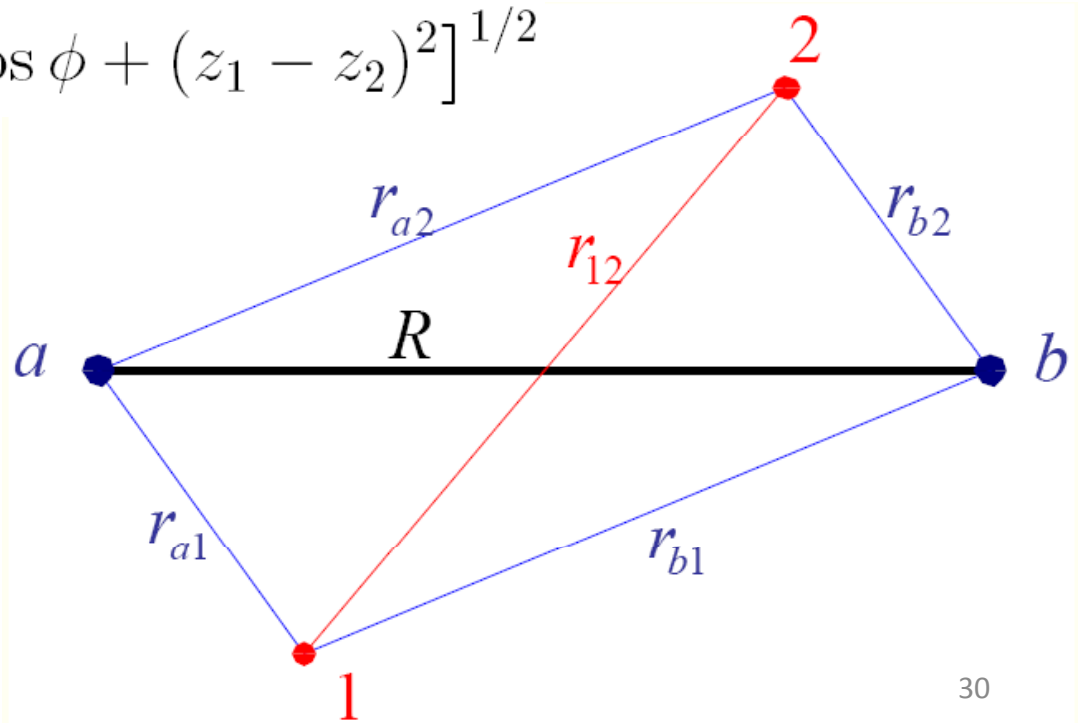


$$V = -\frac{1}{r_{1a}} - \frac{1}{r_{1b}} - \frac{1}{r_{2a}} - \frac{1}{r_{2b}} + \frac{1}{r_{12}} + \frac{1}{R}$$

$$r_{ia} = [\rho_i^2 + (z_i + R/2)^2]^{1/2},$$

$$r_{ib} = [\rho_i^2 + (z_i - R/2)^2]^{1/2},$$

$$r_{12} = [\rho_1^2 + \rho_2^2 - 2\rho_1\rho_2 \cos \phi + (z_1 - z_2)^2]^{1/2}$$



Traditional D -scaling

$$V_{\text{eff}}(\rho_1, z_1, \rho_2, z_2, \phi) = \frac{1}{2} \left(\frac{1}{\rho_1^2} + \frac{1}{\rho_2^2} \right) \frac{1}{\sin^2 \phi} + V(\rho_1, z_1, \rho_2, z_2, \phi)$$

Alternative D -scaling

$$T_\rho = \sum_i \frac{1}{\rho_i^{D-2}} \frac{\partial}{\partial \rho_i} \left(\rho_i^{D-2} \frac{\partial}{\partial \rho_i} \right),$$

$$T_z = \sum_i \frac{\partial}{\partial z_i^2},$$

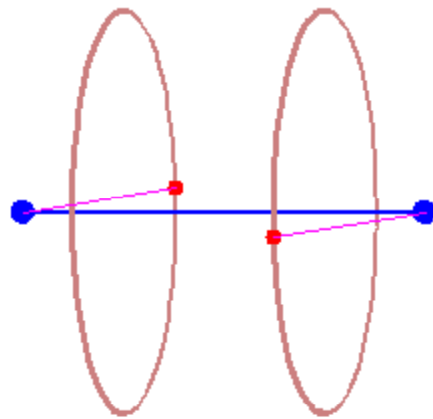
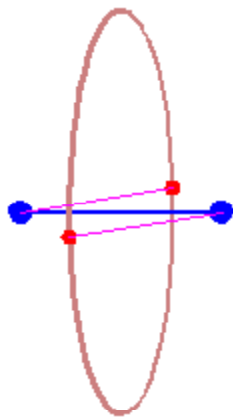
$$T_\phi = \left(\frac{1}{\rho_1^2} + \frac{1}{\rho_2^2} \right) \frac{1}{\sin^{D-3} \phi} \frac{\partial}{\partial \phi} \left(\sin^{D-3} \phi \frac{\partial}{\partial \phi} \right)$$

$$T'_\phi = \left(\frac{1}{\rho_1^2} + \frac{1}{\rho_2^2} \right) \frac{\partial}{\partial \phi} \left(\frac{\partial}{\partial \phi} \right)$$

$$(T_\rho + T_z + T'_\phi + V(\rho_1, z_1, \rho_2, z_2, \phi) - E') \psi(\rho_1, z_1, \rho_2, z_2, \phi) = 0$$

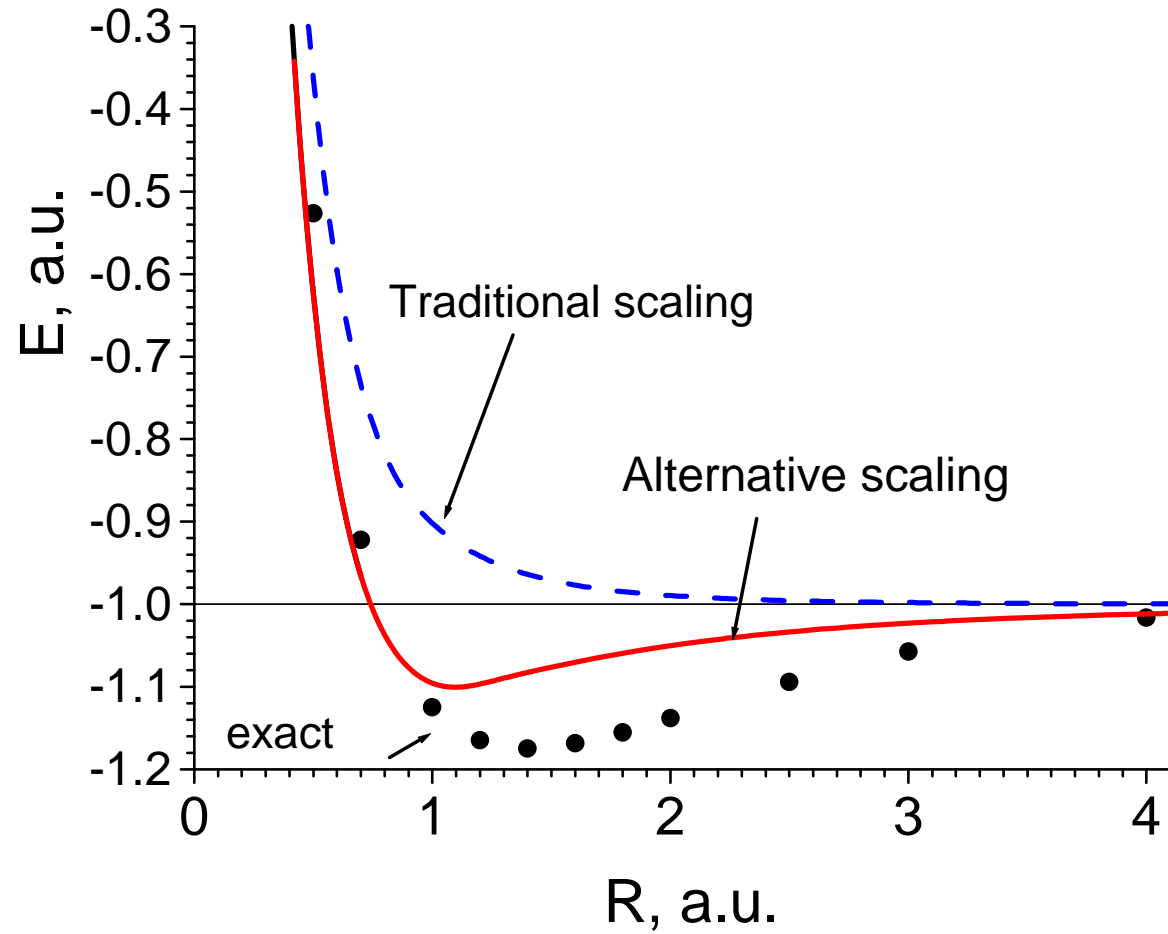
$$V'_{\text{eff}}(\rho_1, z_1, \rho_2, z_2, \phi) = \frac{1}{2} \left(\frac{1}{\rho_1^2} + \frac{1}{\rho_2^2} \right) + V(\rho_1, z_1, \rho_2, z_2, \phi)$$

Classical limit of large D



ground state

Results for H₂



Many-electron atoms

TRADITIONAL VS. ALTERNATIVE D -SCALING FOR TWO-ELECTRON
ATOMS

$$\Psi(\mathbf{r}_1, \mathbf{r}_2) = \psi(r_1, r_2, \theta)$$

$$-\frac{1}{2} (\nabla_1^2 + \nabla_2^2) \Psi(\mathbf{r}_1, \mathbf{r}_2) = T_D \psi(r_1, r_2, \theta) =$$
$$-\frac{1}{2} \left[\frac{1}{r_1^{D-1}} \frac{\partial}{\partial r_1} r_1^{D-1} \frac{\partial}{\partial r_1} + \frac{1}{r_2^{D-1}} \frac{\partial}{\partial r_2} r_2^{D-1} \frac{\partial}{\partial r_2} + \right.$$
$$\left. \left(\frac{1}{r_1^2} + \frac{1}{r_2^2} \right) \frac{1}{\sin^{D-2} \theta} \frac{\partial}{\partial \theta} \sin^{D-2} \theta \frac{\partial}{\partial \theta} \right] \psi(r_1, r_2, \theta)$$

$$(T_3 + V - E_{\text{phys}}) \psi_{\text{phys}} = 0$$

$$V = -\frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{r_{12}}$$

Summary of the traditional method of D -scaling

$$(T_D + V - E_D) \psi_D = 0$$

$$E_D \approx \left(\frac{2}{D-1} \right)^2 \tilde{E}_0$$

$$E_{\text{phys}} \approx \tilde{E}_0$$

$$P(r_1, r_2, \theta) = (r_1 r_2)^{\frac{D-1}{2}} \sin^{\frac{D-2}{2}} \theta \psi(r_1, r_2, \theta)$$

$$\left\{ -\frac{1}{2} \left[\frac{\partial^2}{\partial r_1^2} + \frac{\partial^2}{\partial r_2^2} + \left(\frac{1}{r_1^2} + \frac{1}{r_2^2} \right) \frac{\partial^2}{\partial \theta^2} \right] + \frac{1}{2} \left(\frac{1}{r_1^2} + \frac{1}{r_2^2} \right) \left[\frac{(D-2)(D-4)}{4 \sin^2 \theta} - \frac{1}{4} \right] + V - E_D \right\} P(r_1, r_2, \theta) = 0.$$

scaling transformation

$$r_1 = K^2 \tilde{r}_1, \quad r_2 = K^2 \tilde{r}_2, \quad \text{where } K = \frac{1}{2} \sqrt{(D-2)(D-4)}$$

$$\tilde{U}(\tilde{r}_1, \tilde{r}_2, \theta) = \frac{1}{2 \sin^2 \theta} \left(\frac{1}{\tilde{r}_1^2} + \frac{1}{\tilde{r}_2^2} \right) + V(\tilde{r}_1, \tilde{r}_2, \theta)$$

$$\cos \theta = -\frac{1 + \sqrt{1 + 128Z^2}}{64Z^2}$$

For helium ($Z = 2$), $\cos \theta \approx -\frac{\sqrt{2}}{8Z} \approx -0.09$, and the angle is 95.3°

$$\tilde{E}_0 = -\frac{(1 - \xi)^3}{32\xi^2}, \quad \xi \equiv -\cos \theta$$

Alternative D -scaling for helium

$$T'_D = -\frac{1}{2} \left[\frac{1}{r_1^{D-1}} \frac{\partial}{\partial r_1} r_1^{D-1} \frac{\partial}{\partial r_1} + \frac{1}{r_2^{D-1}} \frac{\partial}{\partial r_2} r_2^{D-1} \frac{\partial}{\partial r_2} + \left(\frac{1}{r_1^2} + \frac{1}{r_2^2} \right) \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta} \right]$$

$$(T'_D + V - E'_D) \psi'_D = 0$$

$$E'_D \approx \left(\frac{2}{D-1} \right)^2 \tilde{E}'_0 \quad E_{\text{phys}} \approx \tilde{E}'_0$$

$$P'(r_1, r_2, \theta) = (r_1 r_2)^{\frac{D-1}{2}} \psi(r_1, r_2, \theta)$$

$$\left\{ -\frac{1}{2} \left[\frac{\partial^2}{\partial r_1^2} + \frac{\partial^2}{\partial r_2^2} + \left(\frac{1}{r_1^2} + \frac{1}{r_2^2} \right) \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta} \right] + \frac{(D-1)(D-3)}{8} \left(\frac{1}{r_1^2} + \frac{1}{r_2^2} \right) + V(r_1, r_2, \theta) - E'_D \right\} P'(r_1, r_2, \theta) = 0.$$

$$r_1 = K'^2 \tilde{r}_1, \quad r_2 = K'^2 \tilde{r}_2, \quad \text{where } K' = \frac{1}{2} \sqrt{(D-1)(D-3)}$$

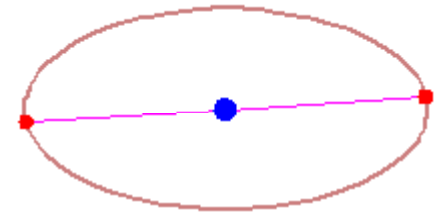
$$\left\{ -\frac{1}{2K'^4} \left[\frac{\partial^2}{\partial \tilde{r}_1^2} + \frac{\partial^2}{\partial \tilde{r}_2^2} + \left(\frac{1}{\tilde{r}_1^2} + \frac{1}{\tilde{r}_2^2} \right) \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta} \right] + \frac{K'^2}{2K'^4} \left(\frac{1}{\tilde{r}_1^2} + \frac{1}{\tilde{r}_2^2} \right) + \frac{1}{K'^2} V(\tilde{r}_1, \tilde{r}_2, \theta) - \frac{1}{K'^2} \tilde{E}'_D \right\} \tilde{P}'(\tilde{r}_1, \tilde{r}_2, \theta) = 0,$$

$$\tilde{E}'_D \equiv K'^2 E'_D$$

$$\left\{ -\frac{1}{2K'^2} \left[\frac{\partial^2}{\partial \tilde{r}_1^2} + \frac{\partial^2}{\partial \tilde{r}_2^2} + \left(\frac{1}{\tilde{r}_1^2} + \frac{1}{\tilde{r}_2^2} \right) \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta} \right] + \frac{1}{2} \left(\frac{1}{\tilde{r}_1^2} + \frac{1}{\tilde{r}_2^2} \right) + V(\tilde{r}_1, \tilde{r}_2, \theta) - \tilde{E}'_D \right\} \tilde{P}'(\tilde{r}_1, \tilde{r}_2, \theta) = 0$$

$$\tilde{U}'(\tilde{r}_1, \tilde{r}_2, \theta) = \frac{1}{2} \left(\frac{1}{\tilde{r}_1^2} + \frac{1}{\tilde{r}_2^2} \right) - \frac{Z}{\tilde{r}_1} - \frac{Z}{\tilde{r}_2} + \frac{1}{\sqrt{\tilde{r}_1^2 + \tilde{r}_2^2 - 2\tilde{r}_1\tilde{r}_2 \cos \theta}}$$

$$\theta = 180^\circ$$



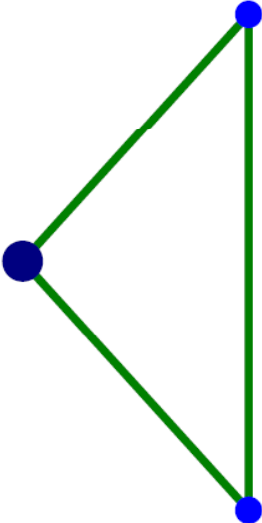

$$\tilde{r}_1 = \tilde{r}_2 \equiv \tilde{r}$$

$$\tilde{r} = \frac{1}{Z - 1/4}$$

$$\tilde{E}'_0 = \frac{1}{(Z - 1/4)^2}$$

Comparison of two approaches

Comparison of two models of helium atom, based on traditional and alternative D -scaling. The second model is reminiscent of pre-quantum Bohr-like model of helium

	Traditional D -scaling	Alternative D -scaling
Configuration		
$\tilde{r}_1 = \tilde{r}_2$	0.607	0.571
\tilde{r}_{12}	0.897	1.143
θ	95.3°	180°
Energy (% error)	-2.738 (-5.7%)	-3.0625 (+5.5%) 40

Many-electron atoms in the limit of large dimensionality

Atomic energies from the large-dimension limit

J. G. Loeser

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(Received 23 December 1986; accepted 11 February 1987)

Analytic approximations to nonrelativistic atomic ground state energies are obtained from the first two terms of the $1/D$ expansion for the N -electron atom. These two terms describe the equilibrium structure ($D \rightarrow \infty$ limit) and normal mode oscillations ($1/D$ term) of a completely symmetric N -dimensional configuration of localized particles. The connection between these large- D results and real atoms is established through the vibrational state, which is restricted by antisymmetry requirements at $D = 3$. Convergence considerations lead us to consider three different approximations, depending on whether all, none, or part of the results obtained from the $1/D$ term are used (in addition to those obtained from the $D \rightarrow \infty$ limit); the maximum errors are respectively about 8%, 3%, and 1%. In all three approximations the dependence of neutral atom energies on the nuclear charge Z is roughly $Z^{12/5}$ for physical Z (as observed for real atoms) and roughly $Z^{7/3}$ for very large Z (in agreement with the known asymptotic result). The best approximation, which utilizes the $1/D$ term up to lowest nonvanishing order in $1/Z$, is comparable in accuracy to single- ζ Hartree-Fock calculations.

Bohr model and dimensional scaling analysis of atoms and molecules

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Alternative D-scaling for many-electron atoms

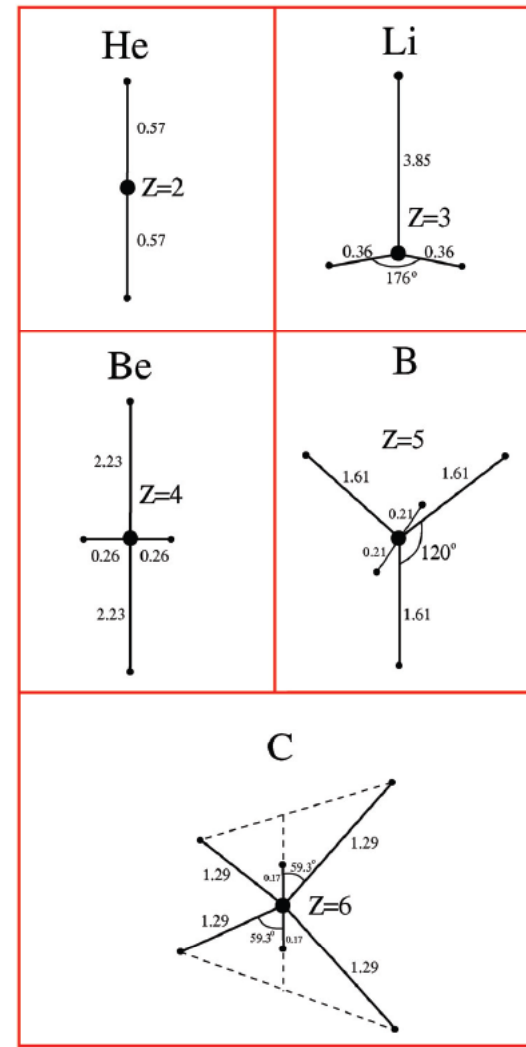
$$E = \frac{1}{2} \sum_{i=1}^N \frac{n_i^2}{r_i^2} + V(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N)$$

Svidzinsky et al. considered minimization in 3D space
(when $\mathbf{r}_1, \dots, \mathbf{r}_N$ have 3 components).

Total number of minimization variables $3N-3$

General theory requires minimization in arbitrary
dimensional space. It lowers the energy.
The total number of variables is only n_{\max}
because of symmetry.

A. Svidzinsky et al.



Electron configurations obtained from Bohr model by minimizing Equation (2.12).
Distances in atomic units (1 a.u. = 0.529 Å).

Comparison of 3D vs. arbitrary D minimization

FLUORINE ATOM - 9 ELECTRONS

F. Dimensionality 3

Energy: $E = -98.0590348$. Shell No. 1 (2 electrons)

$$R = 0.114325952$$

$$R = 0.114327718$$

Shell No. 2 (7 electrons)

$$R = 0.716026787 \text{ (2 electrons)}$$

$$R = 0.735057035 \text{ (2 electrons)}$$

$$R = 0.801661901$$

$$R = 0.805188543$$

$$R = 3.65641704$$

F. Dimensionality 7

Energy: $E = -98.93738$. Shell No. 1 (2 electrons)

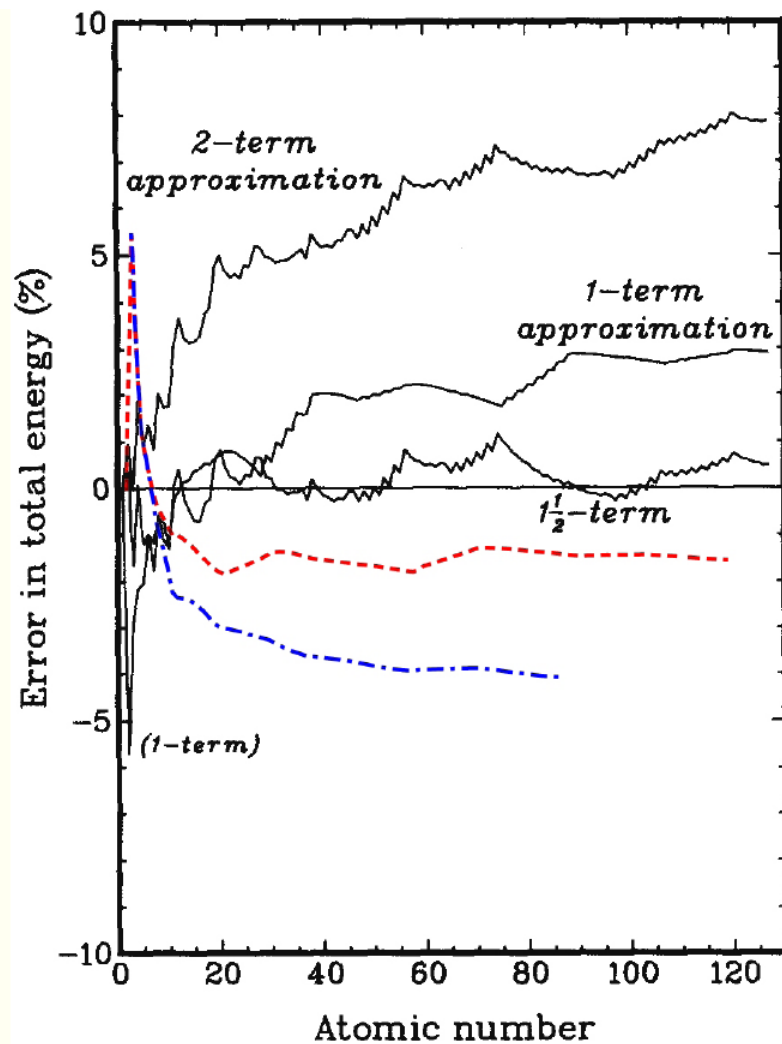
$$R = 0.114562165 \text{ (2 electrons)}$$

Shell No. 2 (7 electrons)

$$R = 0.784569025 \text{ (7 electrons)}$$

For example, for neon atom,

$$W = -\frac{39}{2R_1} + \frac{7\sqrt{7}}{R_2} - \frac{80}{R_2} + \frac{1}{R_1^2} + \frac{16}{R_2^2} + \frac{16}{\sqrt{R_1^2 + 43R_2^2}}$$



Accuracy of Bohr model as a function of Z . Solid lines are approximations introduced in [10]. Dot-dashed line are results of the Bohr model based on a minimization of classical configurations in three dimensional space, and dashed line in multidimensional space.

- [10] J. G. Loeser, *Atomic energies from the large-dimension limit*, J. Chem. Phys. **86** (1987), 5635–5646.

V. COMBINING BOHR MODEL AND THOMAS - FERMI THEORY

According to statistical Thomas - Fermi theory, the energy behaves at large Z as

$$E \sim E^{(Z \rightarrow \infty)} = -0.76875Z^{7/3} + 0.5Z^2 - 0.2699Z^{5/3}, \quad (15)$$

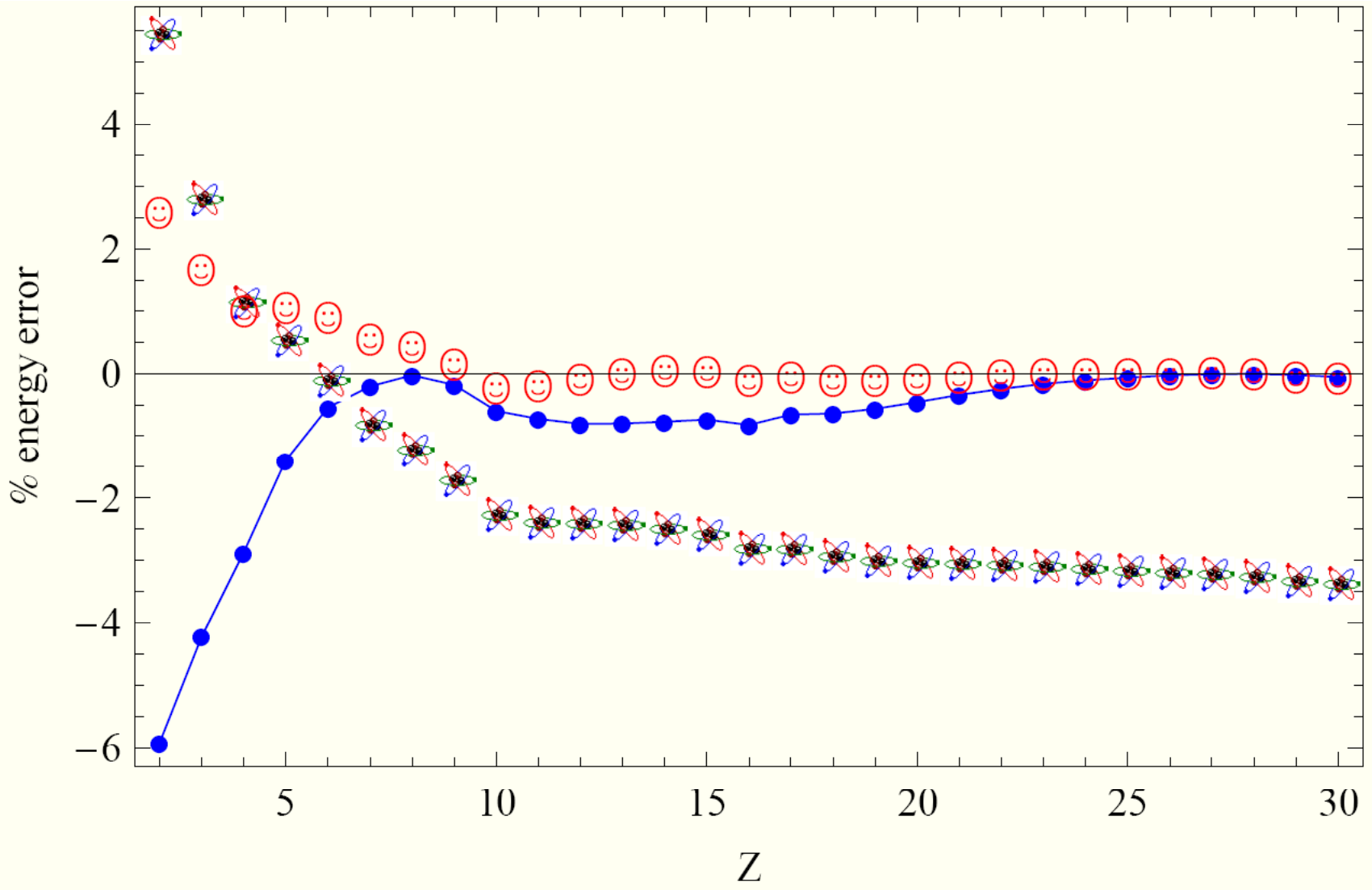
;

Bohr energy has a similar functional behavior at large Z , but with slightly different coefficients,

$$E_{\text{Bohr}} \sim E_{\text{Bohr}}^{(Z \rightarrow \infty)} = C_0Z^{7/3} + C_1Z^2 + C_2Z^{5/3}, \quad (16)$$

$$\epsilon_{\text{TF}} = E^{(Z \rightarrow \infty)} - E_{\text{Bohr}}^{(Z \rightarrow \infty)} = -0.03286Z^{7/3} + 0.0534Z^2 + 0.0199Z^{5/3} \quad (18)$$

$$E_{\text{Bohr-TF}} = E_{\text{Bohr}} + \epsilon_{\text{TF}} \quad (19)$$



Relative errors of Bohr energy (atomic symbols), Thomas-Fermi energy given by equation (15) (filled circles) and combined energy given by equation (19) (happy smileys).

Conclusions

- In the generalized Bohr model for helium, electrons move on stable circular orbits in 4D space and form rigid triangle configuration.
- Alternative D-scaling for atoms requires consideration of arbitrary dimensional configurations of electrons. It gives some improvement in accuracy in comparison with the earlier model in 3D space.
- Combining Bohr model with Thomas-Fermi theory considerably improves accuracy