1.021, 3.021, 10.333, 22.00 : Introduction to Modeling and Simulation : Spring 2011

Part II – Quantum Mechanical Methods : Lecture 3

From Many-Body to Single-Particle: Quantum Modeling of Molecules

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Part II Outline

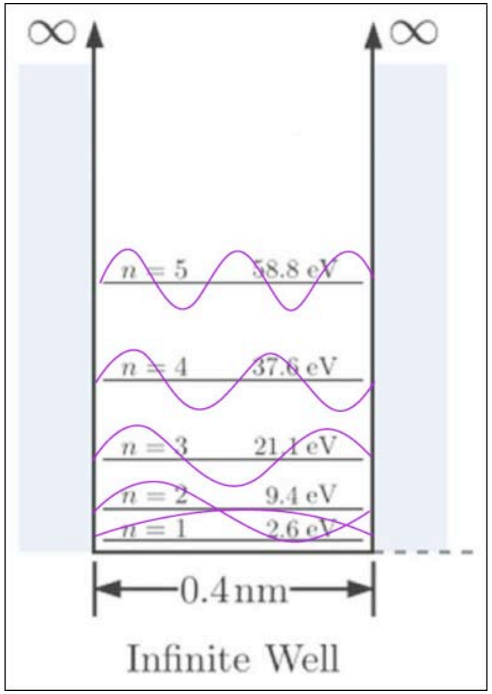
theory & practice

1. It’s A Quantum World: The Theory of Quantum Mechanics
2. Quantum Mechanics: Practice Makes Perfect
3. From Many-Body to Single-Particle; Quantum Modeling of Molecules
4. From Atoms to Solids
5. Quantum Modeling of Solids: Basic Properties
6. Advanced Prop. of Materials: What else can we do?

example applications

7. Nanotechnology
8. Solar Photovoltaics: Converting Photons into Electrons
9. Thermoelectrics: Converting Heat into Electricity
10. Solar Fuels: Pushing Electrons up a Hill
11. Hydrogen Storage: the Strength of Weak Interactions
12. Review

Motivation



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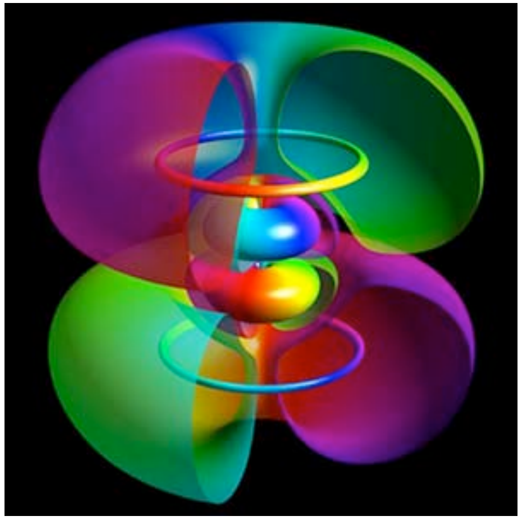
Last time: 1-electron quantum mechanics to describe spectral lines

?
↔

Courtesy ESA and NASA. Image from Wikimedia Commons, http://commons.wikimedia.org.



Courtesy of Bernd Thaller. Used with permission.

Today: many electrons to describe materials.

?
↔

Lesson outline

- Review
- The Many-body Problem
- Hartree and Hartree-Fock
- Density Functional Theory
- Computational Approaches
- Modeling Software
- PWscf

Review: Schrödinger equation

H time independent: $\psi(\vec{r},t) = \psi(\vec{r}) \cdot f(t)$

$$i\hbar \frac{\dot{f}(t)}{f(t)} = \frac{H\psi(\vec{r})}{\psi(\vec{r})} = \text{const.} = E$$

$$\boxed{H\psi(\vec{r}) = E\psi(\vec{r})}$$

$$\psi(\vec{r},t) = \psi(\vec{r}) \cdot e^{-\frac{i}{\hbar}Et}$$

time independent Schrödinger equation
stationary Schrödinger equation

Review: The hydrogen atom

stationary
Schrödinger equation

$$H\psi = E\psi$$

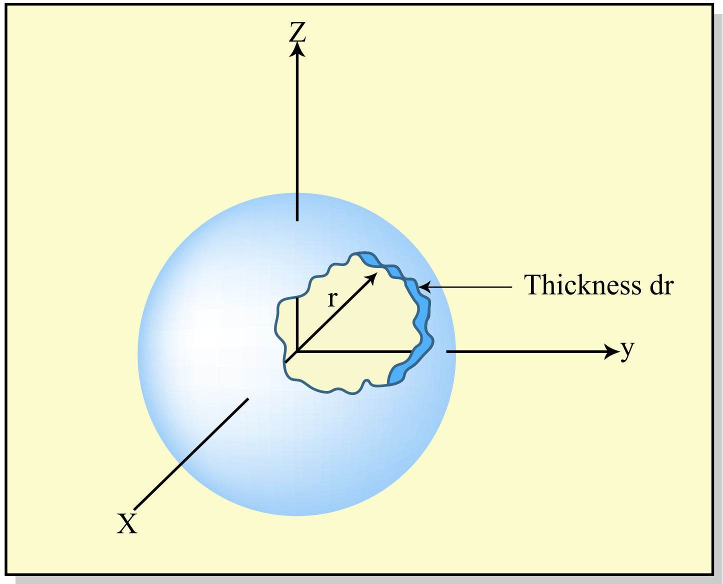
$$\left[T + V \right] \psi = E\psi$$

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V \right] \psi(\vec{r}) = E\psi(\vec{r})$$

just solve
☺

$$\left[-\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\epsilon_0 r} \right] \psi(\vec{r}) = E\psi(\vec{r})$$

Radial Wavefunctions for a Coulomb V(r)



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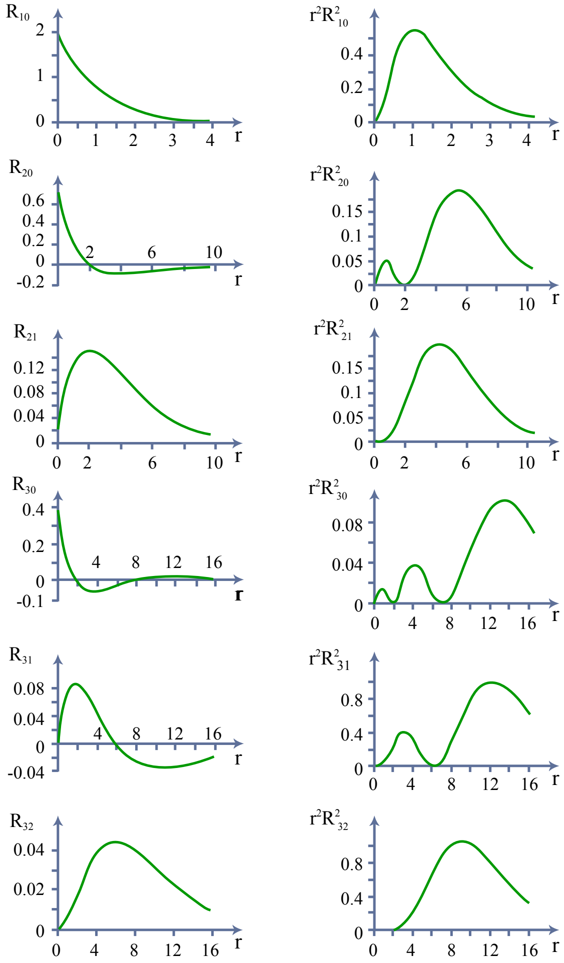


Radial functions $R_{nl}(r)$ and radial distribution functions $r^2R^2_{nl}(r)$ for atomic hydrogen. The unit of length is $a_\mu = (m/_\mu)\, a_0$, where a_0 is the first Bohr radius.

Image by MIT OpenCourseWare.

Angular Parts

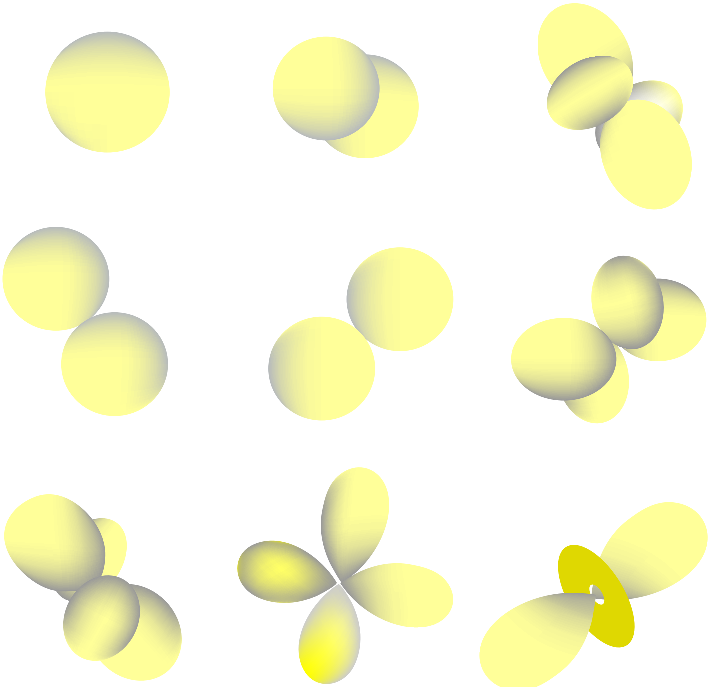


Image by MIT OpenCourseWare.

$$Y_0^0(\theta,\varphi) = \frac{1}{\sqrt{4\pi}}$$

$$Y_1^{\pm 1}(\theta,\varphi) = \mp\sqrt{\frac{3}{8\pi}}\sin\theta e^{\pm i\varphi}$$

$$Y_1^0(\theta,\varphi) = \sqrt{\frac{3}{4\pi}}\cos\theta$$

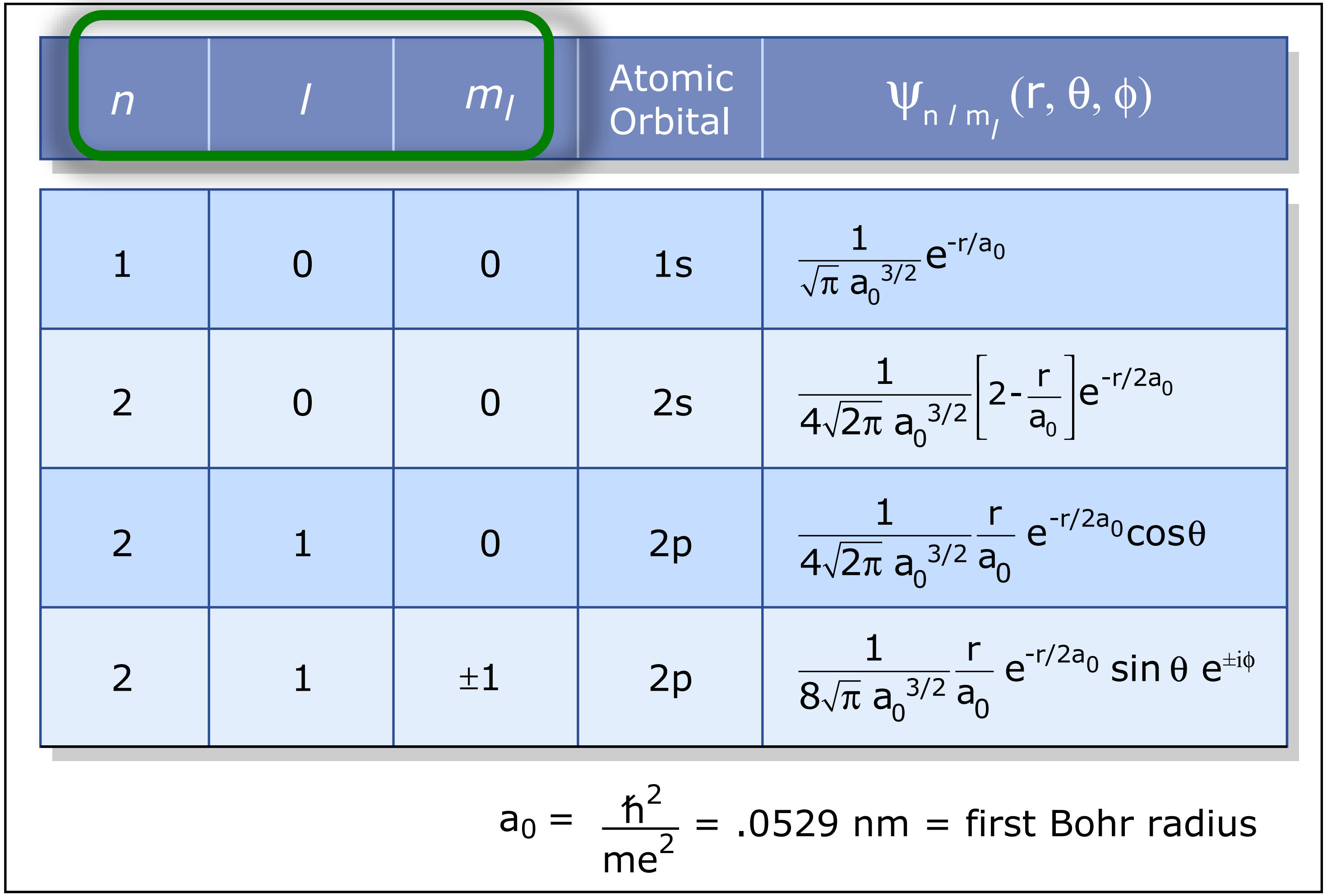
$$Y_2^{\pm 2}(\theta,\varphi) = \sqrt{\frac{15}{32\pi}}\sin^2\theta e^{\pm 2i\varphi}$$

$$Y_2^{\pm 1}(\theta,\varphi) = \mp\sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta e^{\pm i\varphi}$$

$$Y_2^0(\theta,\varphi) = \sqrt{\frac{5}{16\pi}}\left(3\cos^2\theta - 1\right)$$

Review: The hydrogen atom

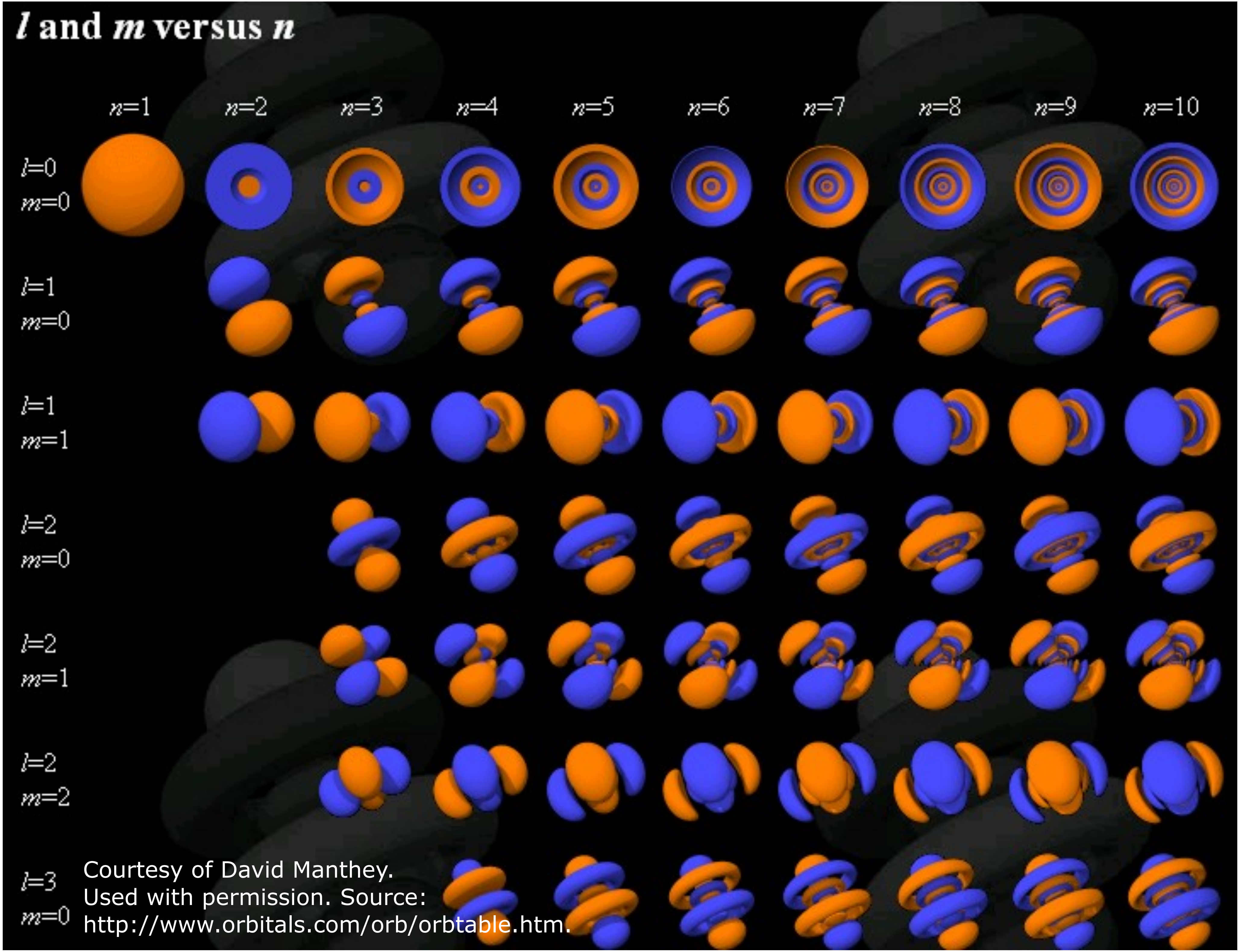
quantum numbers



n	l	m_l	Atomic Orbital	$\psi_{n\,l\,m_l}(r, \theta, \phi)$
1	0	0	1s	$\frac{1}{\sqrt{\pi}\, a_0^{3/2}} e^{-r/a_0}$
2	0	0	2s	$\frac{1}{4\sqrt{2\pi}\, a_0^{3/2}} \left[2-\frac{r}{a_0}\right] e^{-r/2a_0}$
2	1	0	2p	$\frac{1}{4\sqrt{2\pi}\, a_0^{3/2}} \frac{r}{a_0} e^{-r/2a_0} \cos\theta$
2	1	±1	2p	$\frac{1}{8\sqrt{\pi}\, a_0^{3/2}} \frac{r}{a_0} e^{-r/2a_0} \sin\theta\, e^{\pm i\phi}$

$a_0 = \frac{\hbar^2}{me^2}$ = .0529 nm = first Bohr radius

Image by MIT OpenCourseWare.

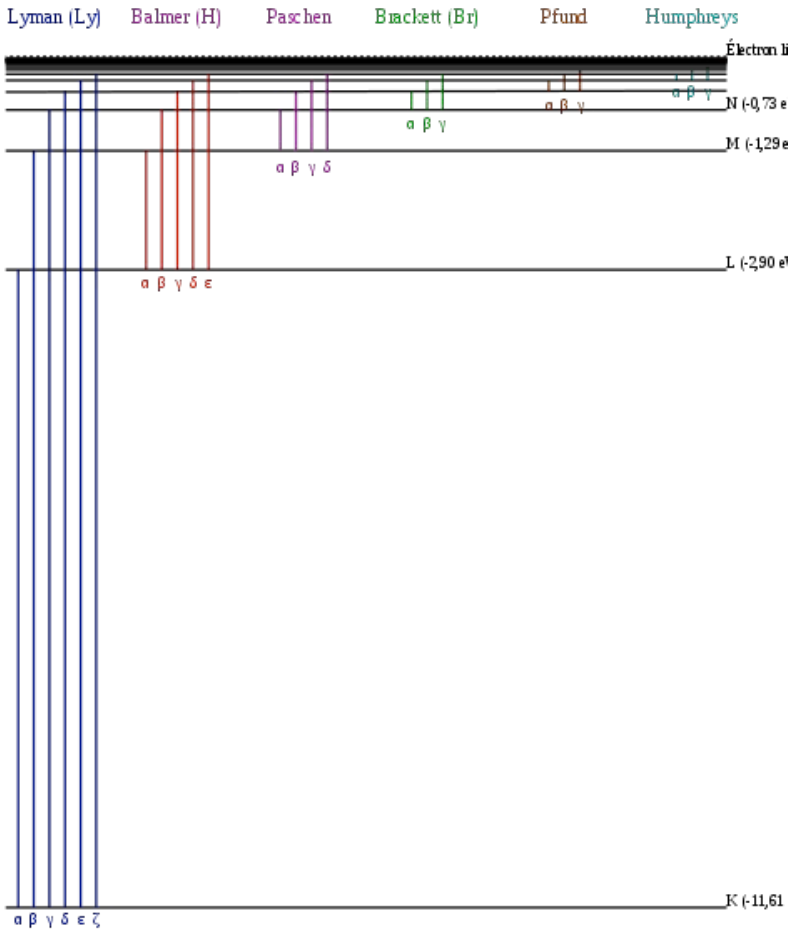


Courtesy of David Manthey.
Used with permission. Source:
http://www.orbitals.com/orb/orbtable.htm.

Review: The hydrogen atom

Please see http://hyperphysics.phy-astr.gsu.edu/hbase/imgmod/hydspe.gif.

Review: The hydrogen atom



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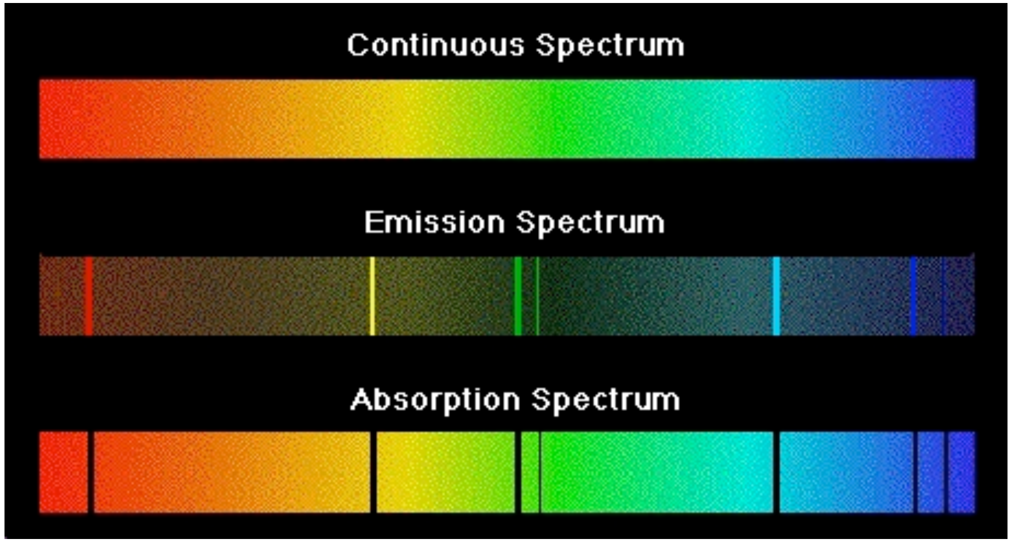
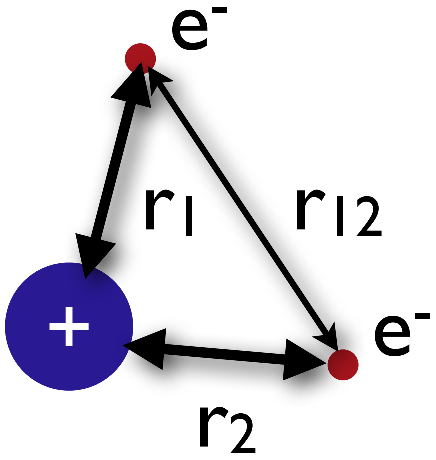


Courtesy of the Department of Physics and Astronomy
at the University of Tennessee. Used with permission.

Review: Next? Helium



$$H\psi = E\psi$$

$$\Big[H_1 + H_2 + W\Big]\psi(\vec{r}_1, \vec{r}_2) = E\psi(\vec{r}_1, \vec{r}_2)$$

$$\Big[T_1 + V_1 + T_2 + V_2 + W\Big]\psi(\vec{r}_1, \vec{r}_2) = E\psi(\vec{r}_1, \vec{r}_2)$$

$$\Big[-\frac{\hbar^2}{2m}\nabla_1^2 - \frac{e^2}{4\pi\epsilon_0 r_1} - \frac{\hbar^2}{2m}\nabla_2^2 - \frac{e^2}{4\pi\epsilon_0 r_2} \boxed{+\frac{e^2}{4\pi\epsilon_0 r_{12}}}\Big]\psi(\vec{r}_1, \vec{r}_2) = E\psi(\vec{r}_1, \vec{r}_2)$$

cannot be solved analytically

problem!

Review: Spin

new quantum number: spin quantum number

for electrons: spin quantum number can ONLY be

up

down

Everything is spinning ...

$$\begin{aligned}\vec{F} &= -\nabla E \\ &= \nabla\, \vec{m} \cdot \vec{B}\end{aligned}$$

Stern–Gerlach experiment (1922)

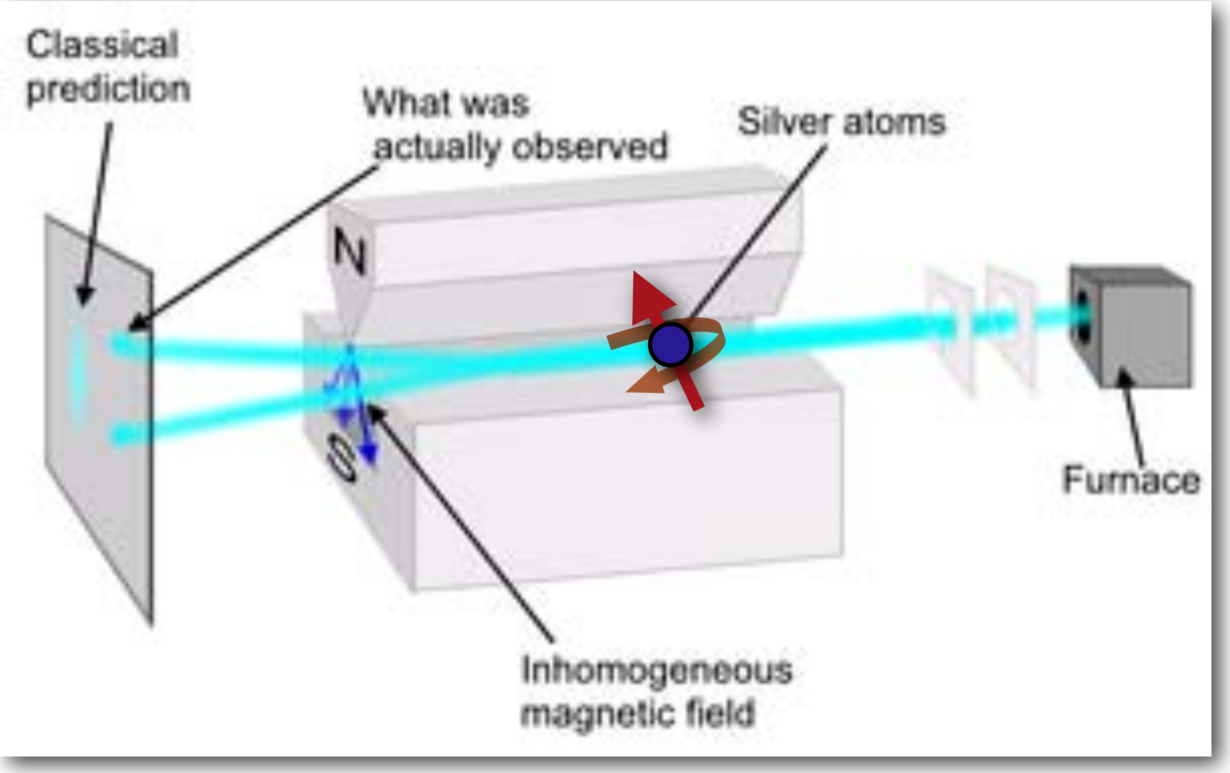
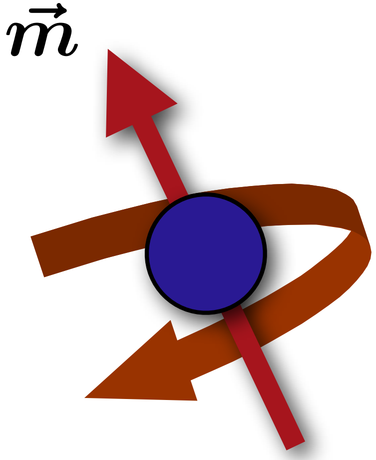


Image courtesy Teresa Knott.

Everything is spinning ...

In quantum mechanics particles can have a magnetic moment and a ”spin”



magnetic moment

$\vec{m}$

spinning charge

Everything is spinning ...

conclusion from the
Stern-Gerlach experiment

for electrons: spin can ONLY be

up

down

Spin History

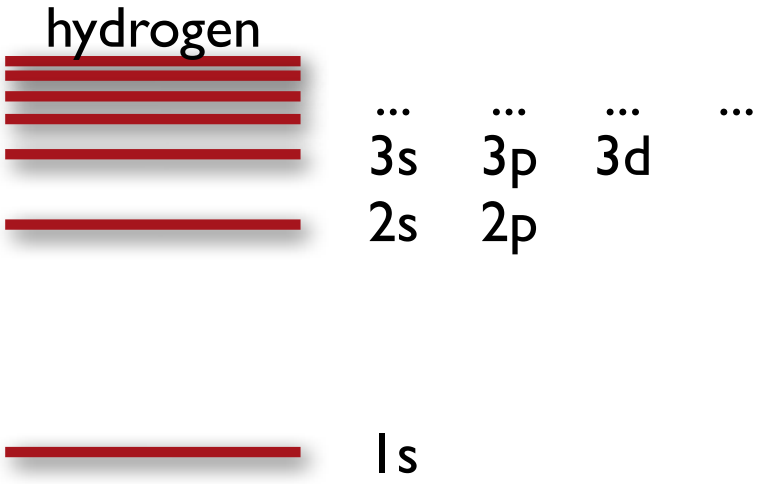
Discovered in 1926 by
Goudsmit and Uhlenbeck

Part of a letter by L. H. Thomas to Goudsmit on March 25, 1926:
http://www.lorentz.leidenuniv.nl/history/spin/thomas.gif.

Pauli's exclusions principle

Two electrons in a system cannot have the same quantum numbers!

quantum numbers:
main n: 1,2,3 ...
orbital l: 0,1,...,n-1
magnetic m: -l,...,l
spin: up, down



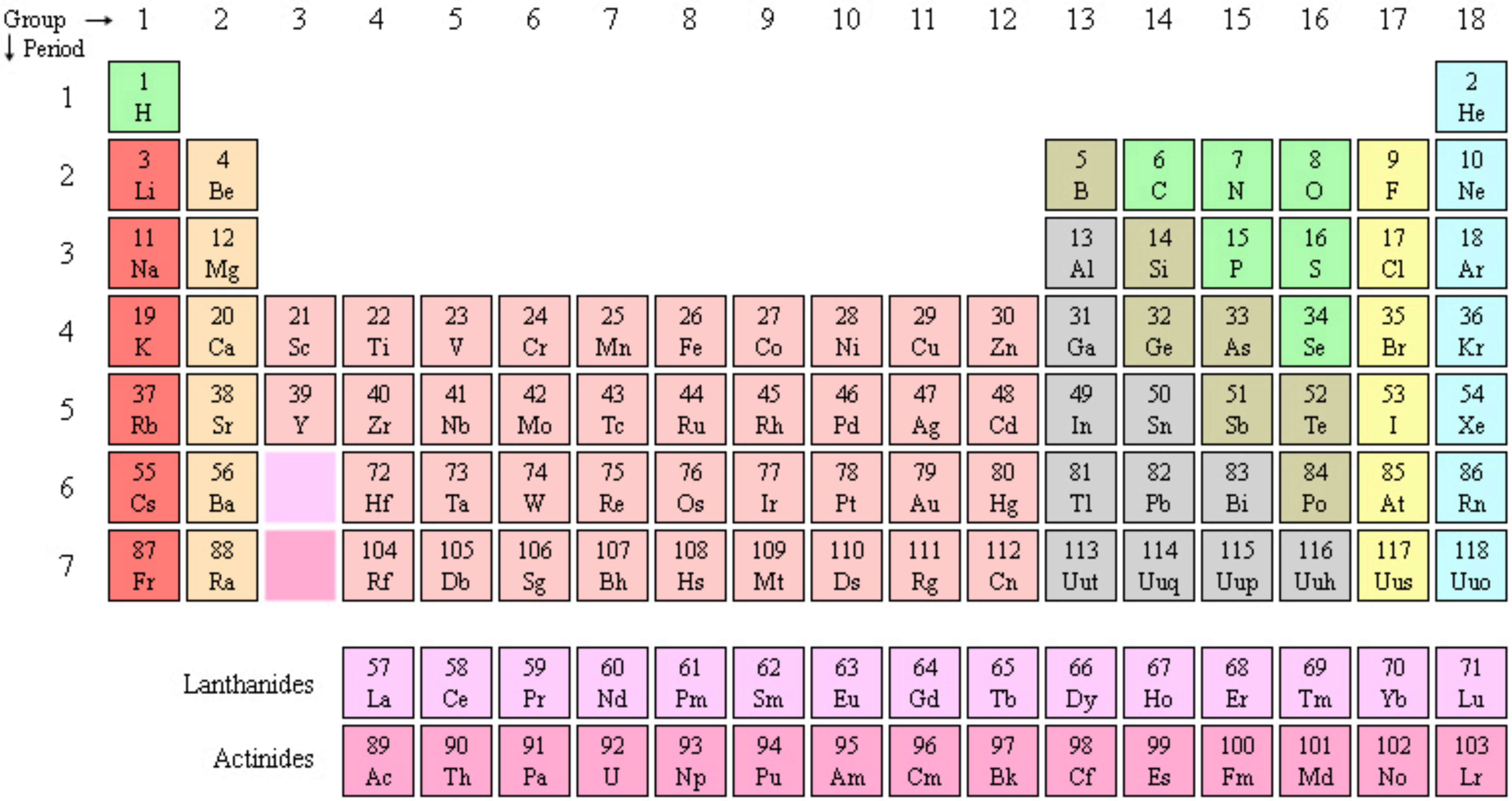
Pauli Exclusion Principle

“Already in my original paper I stressed the circumstance that I was unable to give a logical reason for the exclusion principle or to deduce it from more general assumptions. I had always the feeling, and I still have it today, that this is a deficiency.”

Public domain image.

W. Pauli, Exclusion Principle and Quantum Mechanics, Nobel prize acceptance lecture, Stockholm (1946).

Periodic table



Group → ↓ Period	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	1 H																	2 He
2	3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
3	11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
4	19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
5	37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
6	55 Cs	56 Ba		72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
7	87 Fr	88 Ra		104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Uut	114 Uuq	115 Uup	116 Uuh	117 Uus	118 Uuo
Lanthanides				57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
Actinides				89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr

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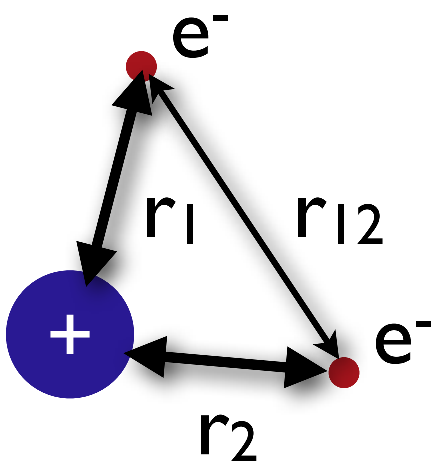
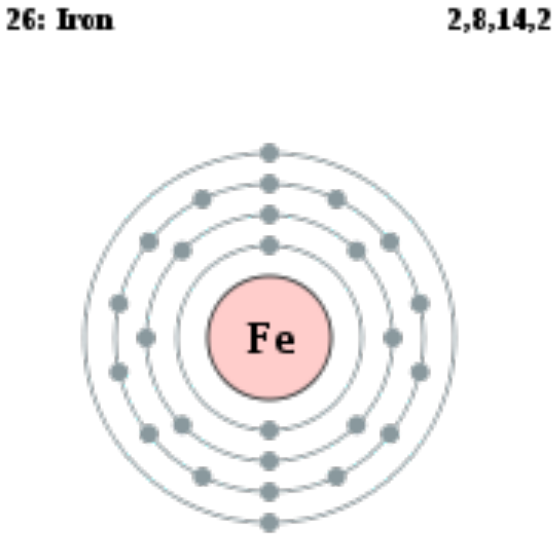
The many-body problem

helium: $2e^-$



iron: $26e^-$



$$\psi = \psi(\vec{r}_1, \ldots, \vec{r}_n)$$

Dirac Quotes

Year 1929…

The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble.

P.A.M. Dirac, Proc. Roy. Soc. 123, 714 (1929)

...and in 1963

If there is no complete agreement […] between the results of one's work and the experiment, one should not allow oneself to be too discouraged [...]

P.A.M. Dirac, Scientific American, May 1963

The Multi-Electron Hamiltonian

$$H\psi = E\psi$$

Remember the good old days of the 1-electron H-atom??

They're over!

$$\left[-\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\epsilon_0 r}\right]\psi(\vec{r}) = E\psi(\vec{r})$$

$$H = \underbrace{-\sum_{i=1}^{N}\frac{h^2}{2M_i}\nabla^2_{\mathbf{R}_i}}_{\text{kinetic energy of ions}} + \underbrace{\frac{1}{2}\sum_{i=1}^{N}\sum_{\substack{j=1\\ i\neq j}}^{N}\frac{Z_iZ_je^2}{\left|\mathbf{R}_i-\mathbf{R}_j\right|}}_{\text{potential energy of ions}} \underbrace{-\frac{h^2}{2m}\sum_{i=1}^{n}\nabla^2_{\mathbf{r}_i}}_{\text{kinetic energy of electrons}} \underbrace{-\sum_{i=1}^{N}\sum_{j=1}^{n}\frac{Z_ie^2}{\left|\mathbf{R}_i-\mathbf{r}_j\right|}}_{\text{electron-electron interaction}} + \underbrace{\frac{1}{2}\sum_{i=1}^{n}\sum_{\substack{j=1\\ i\neq j}}^{n}\frac{e^2}{\left|\mathbf{r}_i-\mathbf{r}_j\right|}}_{\text{electron-ion interaction}}$$

Multi-Atom-Multi-Electron Schrödinger Equation

$$H\left(\mathbf{R}_1,\ldots,\mathbf{R}_N;\mathbf{r}_1,\ldots,\mathbf{r}_n\right)\Psi\left(\mathbf{R}_1,\ldots,\mathbf{R}_N;\mathbf{r}_1,\ldots,\mathbf{r}_n\right) = E\,\Psi\left(\mathbf{R}_1,\ldots,\mathbf{R}_N;\mathbf{r}_1,\ldots,\mathbf{r}_n\right)$$

Born-Oppenheimer Approximation

Screenshot of article removed due to copyright restrictions; see the article online: http://blogs.discovermagazine.com/loom/2009/05/23/sigmas-from-shoulder-to-shoulder-science-tattoos/.

Born-Oppenheimer Approximation (skinless version)

- mass of nuclei exceeds that of the electrons by a factor of 1000 or more
- we can neglect the kinetic energy of the nuclei
- treat the ion-ion interaction classically
- significantly simplifies the Hamiltonian for the electrons:

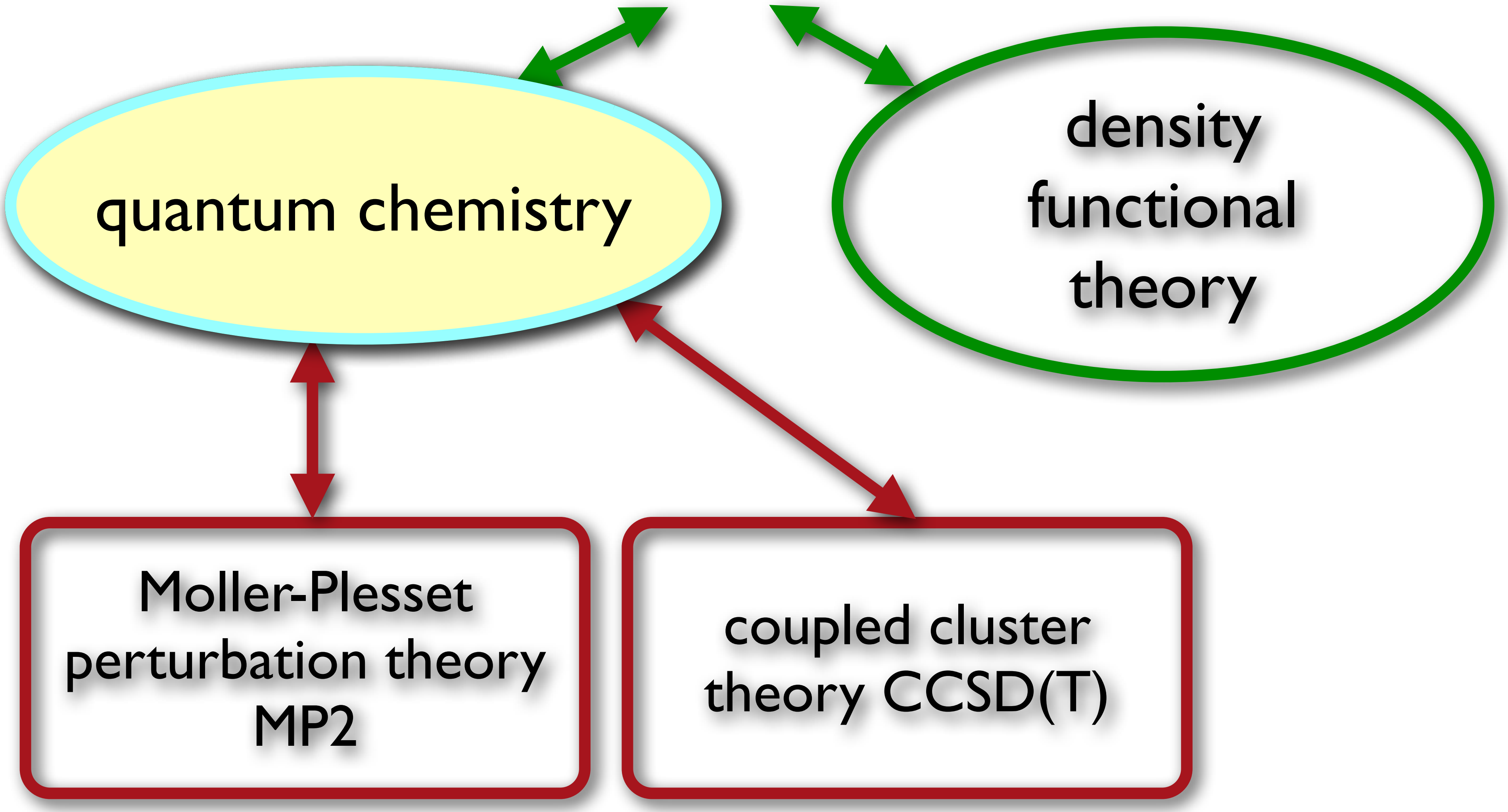

Born


Oppenheimer

This term is just an external potential $V(r_j)$

$$H = -\frac{\hbar^2}{2m}\sum_{i=1}^{n}\nabla_{\mathbf{r}_i}^2 - \sum_{i=1}^{N}\sum_{j=1}^{n}\frac{Z_i e^2}{\left|\mathbf{R}_i - \mathbf{r}_j\right|} + \frac{1}{2}\sum_{i=1}^{n}\sum_{\substack{j=1 \\ i\neq j}}^{n}\frac{e^2}{\left|\mathbf{r}_i - \mathbf{r}_j\right|}$$

Solutions



quantum chemistry

density functional theory

Moller-Plesset perturbation theory MP2

coupled cluster theory CCSD(T)

Hartree Approach

Write wavefunction as a simple product of single particle states:

$$\Psi(\mathbf{r}_1,\ldots,\mathbf{r}_n) = \psi_1(\mathbf{r}_1)\psi_2(\mathbf{r}_2)\ldots\psi_n(\mathbf{r}_n)$$

Hard Product of Easy

Leads to an equation we can solve on a computer!

$$\left\{-\frac{\hbar^2}{2m}\nabla^2 + V_{\mathrm{ext}}(\mathbf{r}) + \sum_{\substack{j=1\\ j\neq i}}^{n}\int d\mathbf{r}\,\frac{e^2\left|\psi_j(\mathbf{r})\right|^2}{\left|\mathbf{r}_j-\mathbf{r}\right|}\right\}\psi_i(\mathbf{r}) = \varepsilon_i\psi_i(\mathbf{r})$$

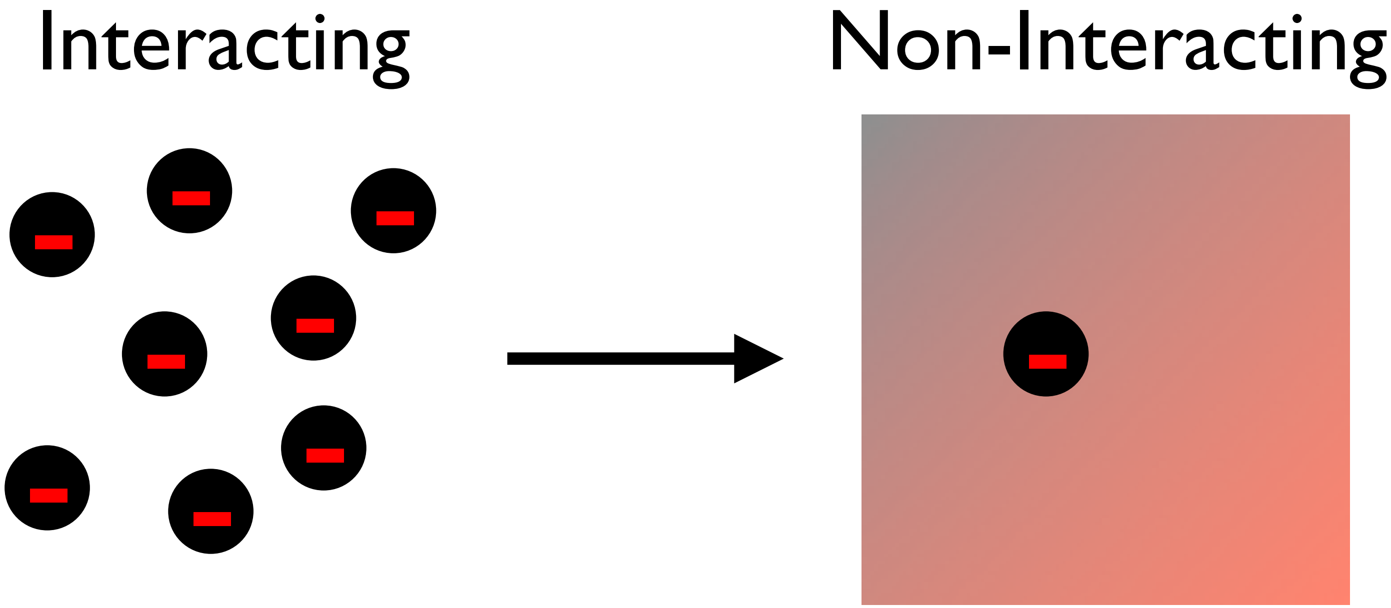
Hartree Approach

$$\left\{-\frac{\hbar^2}{2m}\nabla^2 + V_{\text{ext}}(\mathbf{r}) + \sum_{\substack{j=1\\ j\neq i}}^{n}\int d\mathbf{r}\,\frac{e^2\left|\psi_j(\mathbf{r})\right|^2}{\left|\mathbf{r}_j-\mathbf{r}\right|}\right\}\psi_i(\mathbf{r}) = \varepsilon_i\psi_i(\mathbf{r})$$

The solution for each state depends on all the other states (through the Coulomb term).

- we don’t know these solutions a priori
- must be solved iteratively:
    - guess form for { $\Psi_i^{\text{in}}(\mathbf{r})$ }
    - compute single particle Hamiltonians
    - generate { $\Psi_i^{\text{out}}(\mathbf{r})$ }
    - compare with old
        - if different set { $\Psi_i^{\text{in}}(\mathbf{r})$ } = { $\Psi_i^{\text{out}}(\mathbf{r})$ } and repeat
        - if same, you are done
- obtain the self-consistent solution

Simple Picture...But...



After all this work, there is still one major problem:

the solution is fundamentally wrong

The fix brings us back to spin!

Symmetry Holds the Key

Speculation: everything we know with scientific certainty is somehow dictated by symmetry.

The relationship between symmetry and quantum mechanics is particularly striking.

Exchange Symmetry

- all electrons are *indistinguishable*
  - electrons that made da Vinci, Newton, and Einstein who they were, are *identical* to those within our molecules

    a bit humbling...

- so if
  - I show you a system containing electrons
  - you look away
  - I exchange two electrons in the system
  - you resume looking at system
  - there is no experiment that you can conduct that will indicate that I have switched the two electrons

Mathematically

- define the exchange operator:

$$\chi_{12}\psi_1(r_1)\psi_2(r_2) = \psi_1(r_2)\psi_2(r_1)$$

- exchange operator eigenvalues are ±1:

$$\text{suppose } \hat{\chi}_{12}\,\phi = \chi\phi$$

$$\hat{\chi}_{12}\,\hat{\chi}_{12}\,\phi = \chi^2\phi = \phi$$

$$\chi^2 = 1, \text{ or } \chi = \pm 1.$$

Empirically

- all quantum mechanical states are also eigenfunctions of exchange operators
  - those with eigenvalue 1 (symmetric) are known as Bosons
  - those with eigenvalue -1 (antisymmetric) are known as Fermions
- profound implications for materials properties
  - wavefunctions for our many electron problem must be anti-symmetric under exchange
  - implies Pauli exclusion principle

Hartree-Fock

- Employing Hartree's approach, but
  - enforcing the anti-symmetry condition
  - accounting for spin
- Leads to a remarkable result:

$$\left\{-\frac{\hbar^2}{2m}\nabla^2 + V_{\text{ext}}(\mathbf{r}) + \sum_{\substack{j=1\\ j\neq i}}^{n}\int d\mathbf{r}\,\frac{e^2\left|\psi_j(\mathbf{r})\right|^2}{\left|\mathbf{r}_j-\mathbf{r}\right|}\right\}\psi_i(\mathbf{r}) - \sum_{\substack{j=1\\ j\neq i}}^{n}\delta_{s_i,s_j}\int d\mathbf{r}'\,\frac{e^2}{\left|\mathbf{r}'-\mathbf{r}\right|}\psi_j^*(\mathbf{r}')\psi_i(\mathbf{r}')\psi_j(\mathbf{r}) = \varepsilon_i\psi_i(\mathbf{r})$$

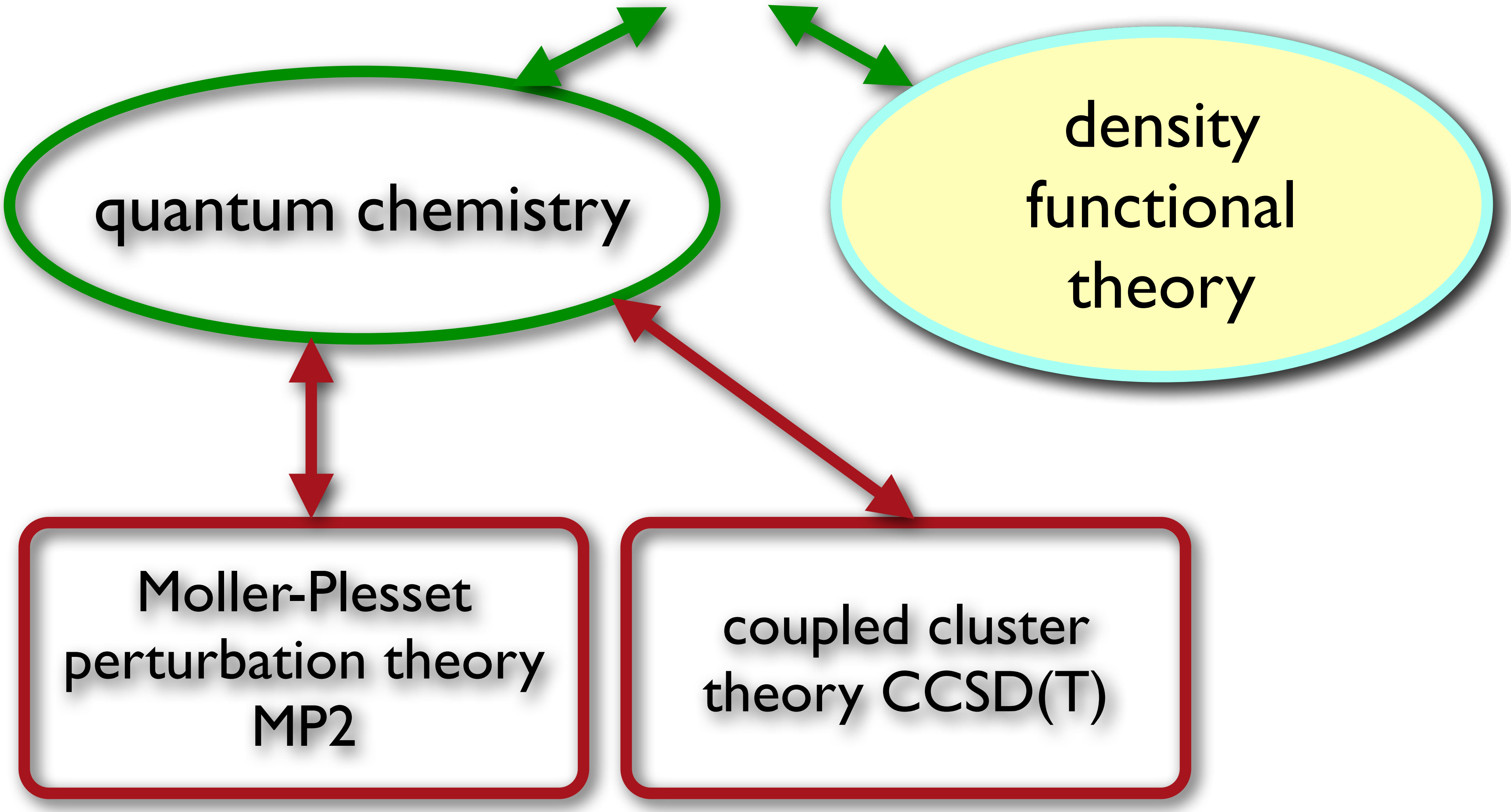
- Hartree-Fock theory is the foundation of molecular orbital theory.
- It is based upon a choice of wavefunction that guarantees antisymmetry between electrons.

it's an emotional moment....

But...Hartree-Fock

- neglects important contribution to electron energy (called “correlation” energy)
- difficult to deal with: integral operator makes solution complicated
- superceded by another approach: density functional theory

Solutions



quantum chemistry

density functional theory

Moller-Plesset perturbation theory MP2

coupled cluster theory CCSD(T)

Solving the Schrodinger Equation

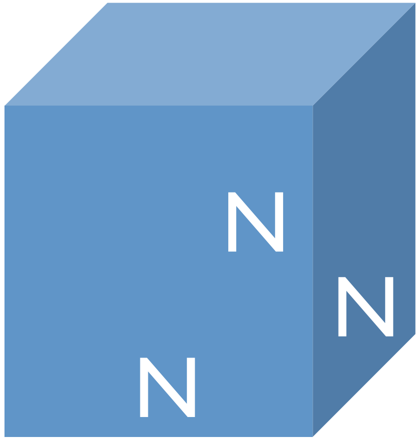
No matter how you slice it, the wavefunction is a beast of an entity to have to deal with.

For example: consider that we have n electrons populating a 3D space.

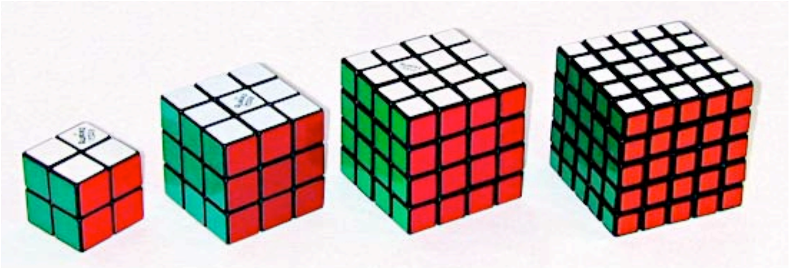
Let’s divide 3D space into NxNxN=2x2x2 grid points.

To reconstruct $\Psi(r)$, how many points must we keep track of?

Solving the Schrodinger Eq.



divide 3D space into NxNxN=2x2x2 grid points



$\Psi = \Psi(r_1, \ldots, r_n)$ # points = N^{3n}

n=# electrons	$\Psi(N^{3n})$
1	8
10	10^9
100	10^{90}
1,000	10^{900}

Working with the Density

The electron density seems to be a more manageable quantity.

Wouldn’t it be nice if we could reformulate our problem in terms of the density, rather than the wavefunction?

Energy ↔ Electron Density

$$E_0=E[n_0]$$

Why DFT?

computational expense
for system size N:

Quantum Chemistry methods; MP2, CCSD(T) → $O(N^5\text{-}N^7)$

Density Functional Theory → $O(N^3)$; $O(N)$

Example

silicon
2 atoms/unit cell

DFT: 0.1 sec

MP2: 0.1 sec

CCSD(T): 0.1 sec

silicon
100 atoms/unit cell

DFT: 5 hours

MP2: 1 year

CCSD(T): 2000 years!!!

Why DFT?

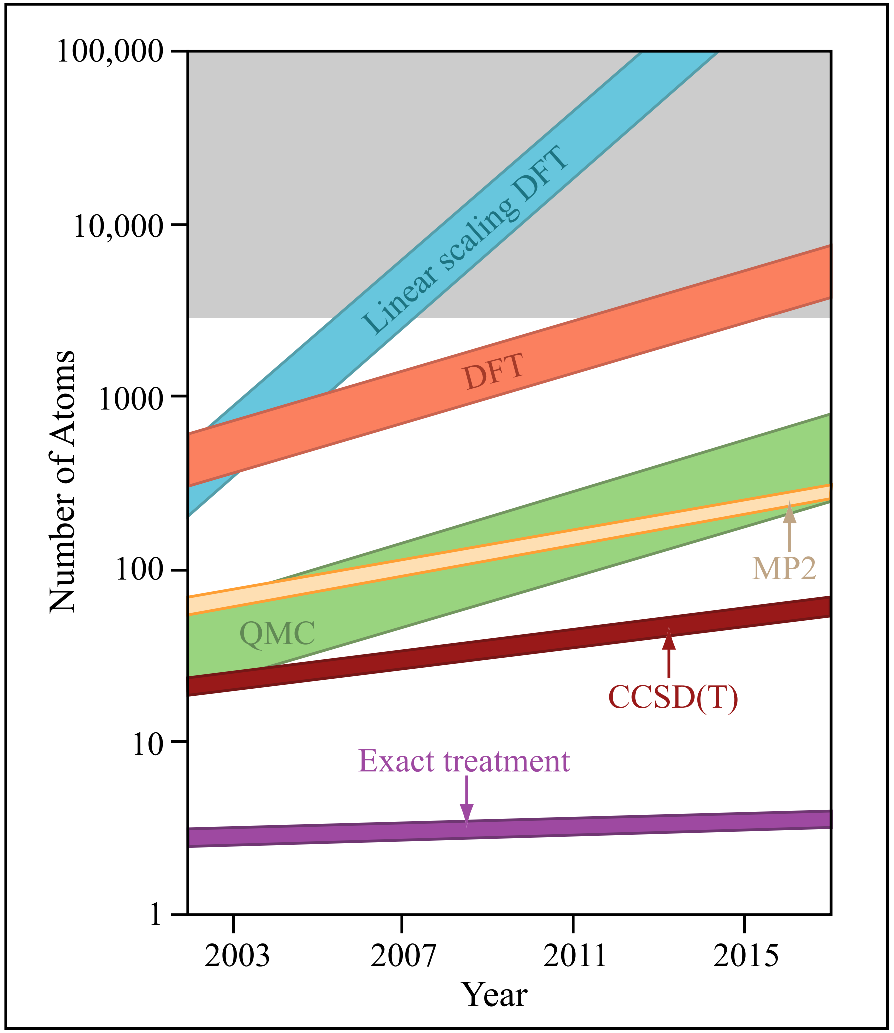


Image by MIT OpenCourseWare.

Density functional theory

$$\psi = \psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N)$$

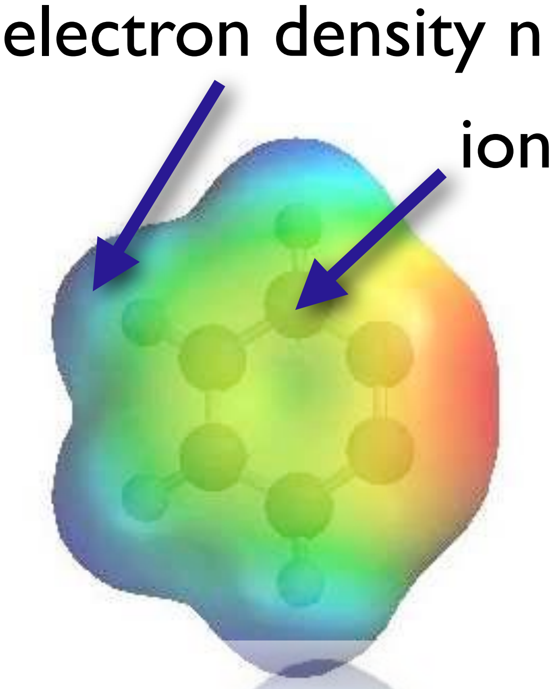
wave function:
complicated!

$$n = n(\vec{r})$$

electron
density:
easy!

Walter Kohn
DFT, 1964

Density functional theory



Total energy is a functional
of the electron density.

$$E[n] = \underbrace{T[n]}_{\text{kinetic}} + \underbrace{V_{ii}}_{\text{ion-ion}} + \underbrace{V_{ie}[n]}_{\text{ion-electron}} + \underbrace{V_{ee}[n]}_{\text{electron-electron}}$$

Density functional theory

$$\boldsymbol{E[n] = \underbrace{T[n]}_{\text{kinetic}} + \underbrace{V_{ii}}_{\text{ion-ion}} + \underbrace{V_{ie}[n]}_{\text{ion-electron}} + \underbrace{V_{ee}[n]}_{\text{electron-electron}}}$$

electron density $\boldsymbol{n(\vec{r}) = \sum_i |\phi_i(\vec{r})|^2}$

$$\boldsymbol{E_{\text{ground state}} = \min_{\phi} E[n]}$$

Find the wave functions that minimize the energy using a functional derivative.

Density Functional Theory

Finding the minimum leads to
Kohn-Sham equations

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V_s(\vec{r})\right]\phi_i(\vec{r}) = \epsilon_i\phi_i(\vec{r}),$$

$$V_s = V + \int \frac{e^2 n_s(\vec{r}\,')}{|\vec{r}-\vec{r}\,'|}\mathrm{d}^3 r' + V_{\mathrm{XC}}[n_s(\vec{r})],$$

ion potential

Hartree potential

exchange-correlation potential

equations for non-interacting electrons

Density functional theory

$$V_s = V + \int \frac{e^2 n_s(\vec{r}\,')}{|\vec{r} - \vec{r}\,'|} \mathrm{d}^3 r' + V_{\mathrm{XC}}[n_s(\vec{r})],$$

Only one problem: v_{xc} not known!

approximations necessary

local density
approximation
LDA

general gradient
approximation
GGA

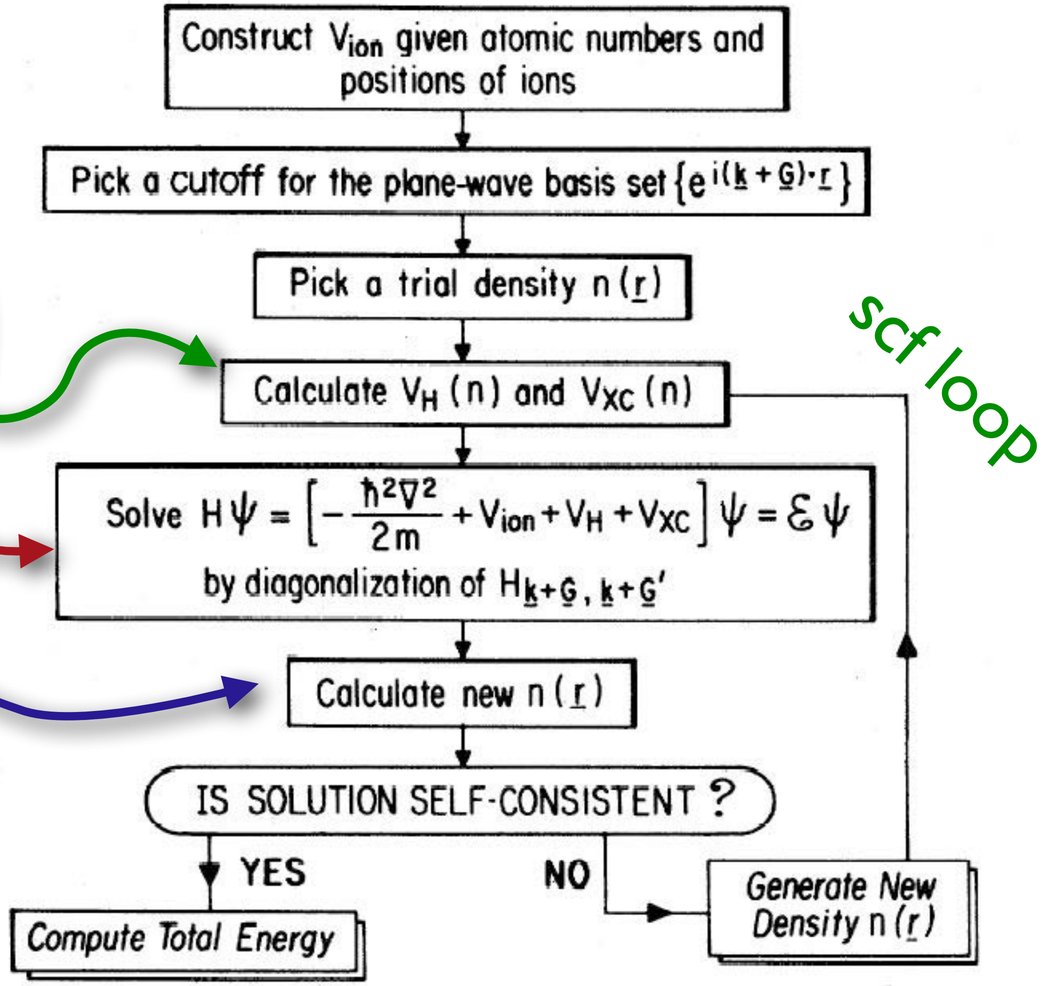
Self-consistent cycle

Kohn-Sham equations

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V_s(\vec{r})\right]\phi_i(\vec{r}) = \epsilon_i\phi_i(\vec{r}),$$

$$V_s = V + \int \frac{e^2 n_s(\vec{r}\,')}{|\vec{r} - \vec{r}\,'|}\mathrm{d}^3r' + V_{\mathrm{XC}}[n_s(\vec{r})],$$

$$n(\vec{r}) = \sum_i |\phi_i(\vec{r})|^2$$



Modeling software

name	license	basis functions	pro/con
ABINIT	free	plane waves	very structured
ONETEP	pay	Wannier functions	linear scaling
Wien2k	pay	Y_{lm} + plane waves	very accurate
VASP	pay	plane waves	fast
PWscf	free	plane waves	fast

Basis functions

Matrix eigenvalue equation:

$$\psi = \sum_i c_i \phi_i$$

expansion in orthonormalized basis functions

$$H\psi = E\psi$$

$$H \sum_i c_i \phi_i = E \sum_i c_i \phi_i$$

$$\int d\vec{r}\, \phi_j^* H \sum_i c_i \phi_i = E \int d\vec{r}\, \phi_j^* \sum_i c_i \phi_i$$

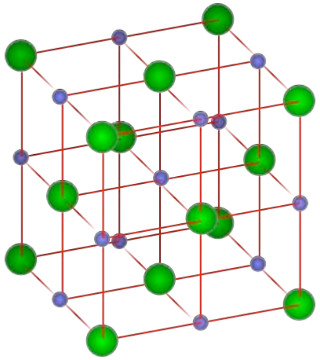
$$\sum_i H_{ji} c_i = E c_j$$

$$\mathcal{H}\vec{c} = E\vec{c}$$

Plane waves as basis functions

plane wave expansion: $$\psi(\vec{r}) = \sum_j c_j \underset{\text{plane wave}}{\boxed{e^{i\vec{G}_j\cdot\vec{r}}}}$$

Cutoff for a maximum G is necessary and results in a finite basis set.



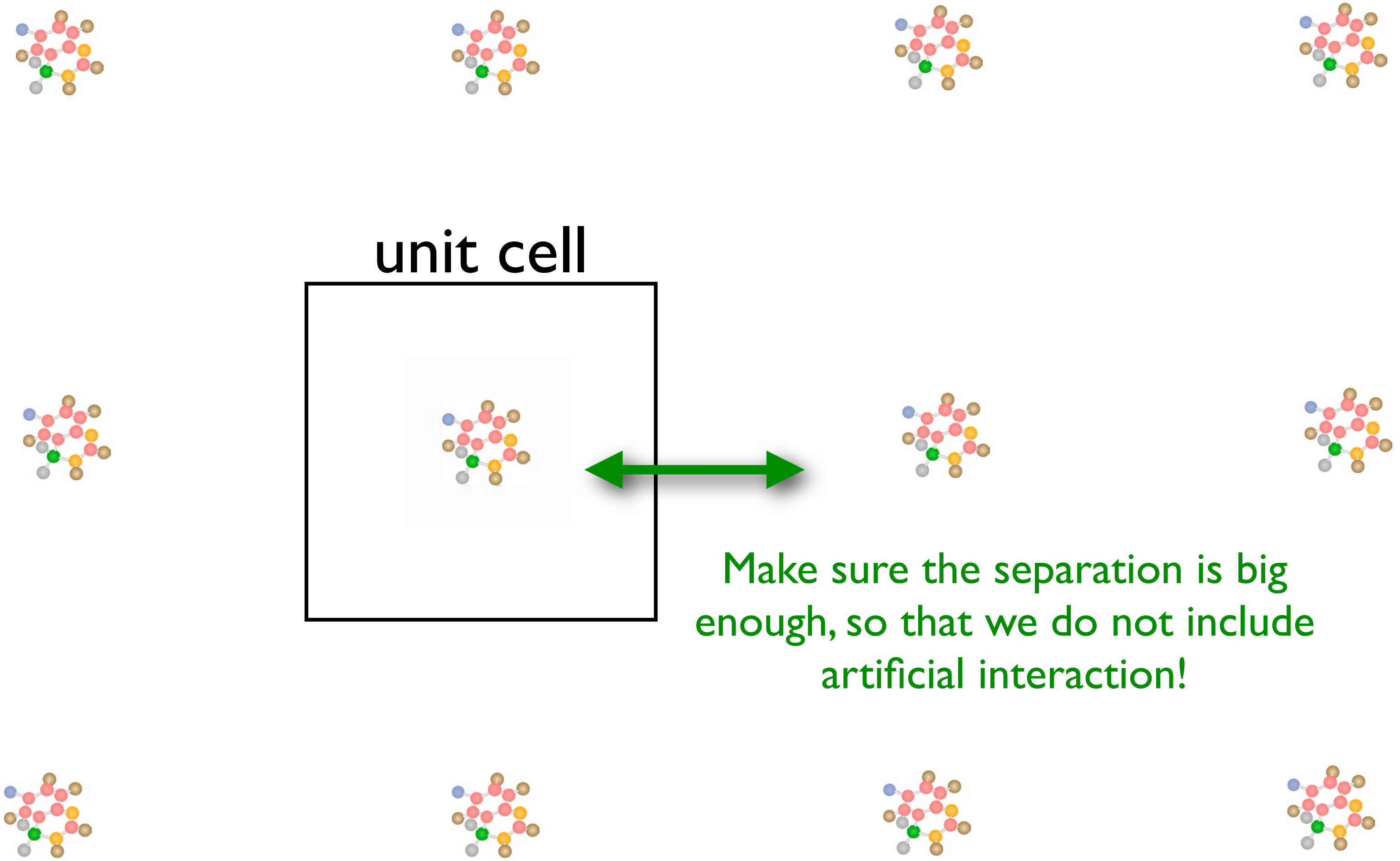
Plane waves are periodic,
thus the wave function is periodic!

Image by MIT OpenCourseWare.

periodic crystals:
Perfect!!! (next lecture)

atoms, molecules:
be careful!!!

Put molecule in a big box



unit cell

Make sure the separation is big enough, so that we do not include artificial interaction!

Images by MIT OpenCourseWare.

DFT calculations

scf loop

```
total energy =   -84.80957141 Ry
total energy =   -84.80938034 Ry
total energy =   -84.81157880 Ry
total energy =   -84.81278531 Ry
total energy =   -84.81312816 Ry
total energy =   -84.81322862 Ry
total energy =   -84.81323129 Ry
```

exiting loop;
result precise enough

At the end we get:

1) electronic charge density

2) total energy

- structure
- bulk modulus
- shear modulus
- elastic constants
- vibrational properties
- sound velocity

☐ binding energies
☐ reaction paths
☐ forces
☐ pressure
☐ stress
☐ ...

Convergence

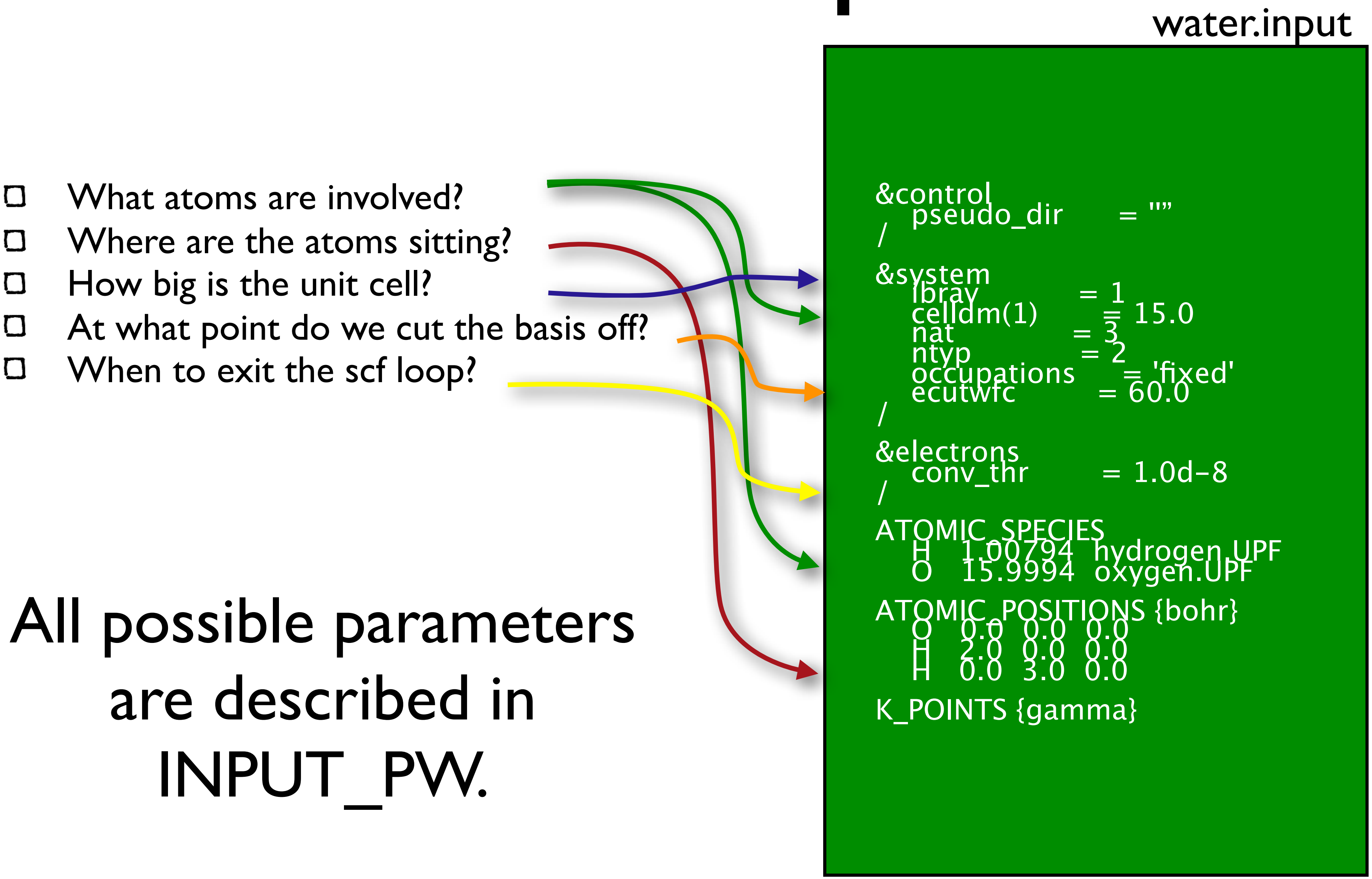
Was my box big enough?

?

Was my basis big enough?

Did I exit the scf loop at the right point?

PWscf input



- ☐ What atoms are involved?
- ☐ Where are the atoms sitting?
- ☐ How big is the unit cell?
- ☐ At what point do we cut the basis off?
- ☐ When to exit the scf loop?

water.input

```
&control
   pseudo_dir      = ""
/
&system
   ibrav           = 1
   celldm(1)       = 15.0
   nat             = 3
   ntyp            = 2
   occupations     = 'fixed'
   ecutwfc         = 60.0
/
&electrons
   conv_thr        = 1.0d-8
/
ATOMIC_SPECIES
   H   1.00794  hydrogen.UPF
   O   15.9994  oxygen.UPF
ATOMIC_POSITIONS {bohr}
   O   0.0  0.0  0.0
   H   2.0  0.0  0.0
   H   0.0  3.0  0.0
K_POINTS {gamma}
```

All possible parameters are described in INPUT_PW.

Review

- Review
- The Many-body Problem
- Hartree and Hartree-Fock
- Density Functional Theory
- Computational Approaches
- Modeling Software
- PWscf

Literature

- Richard M. Martin, Electronic Structure
- Kieron Burke, The ABC of DFT chem.ps.uci.edu/~kieron/dft/
- wikipedia, "many-body physics", "density functional theory", "pwscf", "pseudopotentials", ...

3.021J / 1.021J / 10.333J / 18.361J / 22.00J Introduction to Modeling and Simulation
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