Energetics of isolated d-electron atom

Textbook (old fashioned) J.C. Slater, Quantum Theory of Atomic Structure

* Here: neglect spin orbit coupling

\[ H_{\text{Atom}} = \sum_i -\frac{1}{2m} \frac{\hbar^2}{\lambda_i^2} - \frac{2Ze^2}{r_i} + \frac{i}{2} \sum_{ij} \frac{e^2}{|r_i - r_j|} \]

N el atom: N-body problem. No exact soln.

- Convenient dimensionless units
  \[ \bar{r} = a_B \bar{x}, \quad a_B = \text{Bohr radius} \]
  Energy: Rydberg
  \[ \frac{\varepsilon^2}{2a_B} = 13.6 \text{eV} \]

\[ H_{\text{Atom}} \left[ \text{Ry} \right] = -\sum_i \frac{\hbar^2}{2m} \frac{1}{x_i^2} + \sum_{ij} \frac{d}{|x_i - x_j|} \]

- Conserved quantities: \( N, L_{\text{tot}}, S_{\text{tot}} \Rightarrow E(N, L, S) \)
  In principle, this is all you can say. Just go of best algorithm to solve \( H \)

- Density functional theory

- Hohenberg-Kohn-Sham: F functional \( F(\rho(r)) \) of electron density such that g.s. of H atom optimizes has \( F \) numerics \( \mathcal{F} \) and \( \mathcal{F}(\psi(r)) \Rightarrow \psi_{\text{gs}} \)

- Procedure: auxiliary schr eqn

\[ H_{\text{KS}}: \left[ -\nabla^2 - \frac{2Z}{x} + 2 \int d^3x' \frac{\rho(x')}{|x - x'|} \right] \psi_n(x) + \int d^3x' V_{xc}(x,x') \psi_n(x') \psi_m(x) = E_n \psi_n(x) \]

Find \( N \) lowest eigenvalues

\[ E = \sum_n E_n \]

Issue: form of "exchange-correlation" pot \( V_{xc}(x,x') \)
No theory - various approx forms. Basic workhorse, CMP + quantum chemistry
- Fundamental ambiguity: SIC (self-interaction correction) direct coulomb term here includes \( nz^2 \) of \( e^{-1/z} \) itself. Many forms of \( V_{xc} \) do also. Need to correct.

- Not problematic: solid \( v/10^{23} \) e\(^-\) in extended states.

**Problematic:** atoms, TMO where d-orb. relatively localized

**Alternative approach:** (high degree of acc. cumbersome)

- Hartree-Fock + "CI" (Configuration Interaction)

Here: HF [physical intuition, notation, connects literature]

1. Choose complete set of orthonormal orbitals \( \phi_i^0(x) \)

   Def. \( N \)-pixel state \( \psi(\eta_0, \ldots) = \text{Antisym} \left[ \phi_1^0, \phi_2^0, \ldots, \phi_N^0 \right] \)

   \( \psi = d^{+}_N \psi_0, \ldots, d^{+}_1 \psi_0 \) say \( d^{+}_J \psi \), create electron into state \( J \), spin \( \psi \).

Matrix elt \( H \) bet. 2 seas \( N \) ptrl. det's.

\[
H = \sum_{j=1}^{N} \sum_{\eta_0} \sum_{\eta_1} T_{ij} \delta^{+}_{\eta_0} \delta^{-}_{\eta_1} + \sum_{ijkl} \sum_{\eta_0} \sum_{\eta_1} U_{ijkl} \delta^{+}_{\eta_0} \delta^{-}_{\eta_1} \delta^{+}_{\eta_2} \delta^{-}_{\eta_3}
\]

\[
T_{ij} = \int d^3x \, \phi_i^0(x) \left[ -\nabla^2 - \frac{2z^2}{1x} \right] \phi_j^0(x)
\]

\[
U_{ijkl} = \int d^3x \int d^3y \, \phi_i^0(x) \phi_j^0(y) \phi_k^0(y) \phi_l^0(x) / \lvert x - y \rvert
\]

**Note:** values of mat. elt. \( T_{ij}, U_{ijkl} \) dep. \& on choice of basis.

**Note:** Exact G.S. - superpos of many det

HF: choose \( l \), optimize \( \phi \), CI: correct this.
\[ E_{HF} = \sum_{i} T_{ii} + \sum_{\sigma \sigma'} \frac{1}{2} U_{\sigma \sigma'}^{ijij} + \frac{1}{2} \sum_{\sigma \sigma'} V_{\sigma \sigma'}^{ijij} \sigma_{\sigma i} \sigma_{\sigma' j} \]

Choose occ. orb to min \( E_{HF} \), optimize over normalized \( \phi \)'s: \( \phi_{i0} \)

\[ E_{HF} = \sum_{i} \epsilon_{i0} \left[ \int d^3x |\phi_{i0}(x)|^2 \right] \]

Lagrange multipliers.

\[ \frac{\delta E_{HF}}{\delta \phi_{i0}} = 0 \Rightarrow \epsilon_{i0} \phi_{i0}(x) = \left[ -\nabla^2 - \frac{2Z}{|x|} \right] \phi_{i0}(x) \]

\[ + \sum_{j \neq i} \int d^3y \frac{\phi_{j0}(y)}{|x-y|} \phi_{i0}(x) \]

\[ + \sum_{j} \int d^3y \frac{\phi_{i0}^*(y) \phi_{j0}(x) \phi_{i0}(y)}{|x-y|} \]

These are \( N \) coupled nonlinear eqns.

General statement "Koopmans' Theorem": Lagrange multiplier \( \epsilon_{i0} \) is energy to remove electron from orbital \( i0 \) keeps everything else fixed [in real life, everything else never stays fixed]

Convenient choice of basis: eigenfunctions of \( L_z, L^2 \)

\[ \phi_i(x) = \psi_{n}(1x1) Y_{LM}(x) \]

\[ L^2 Y_{LM} = (L^2 + L) Y_{LM} \]

\[ L_z Y_{LM} = m \ Y_{LM} \]

\[ \sum_{m=-L}^{L} Y_{LM}(x) Y_{LM}(x \cdot \cdot \cdot) = \left( \frac{2L+1}{4\pi} \right)^{1/2} \]

\[ \int d^3x \ Y_{LM}(x)^2 = 1 \]

\[ P_L(1) = 1 \]

\[ \sum_{L=0}^{\infty} \sum_{M=-L}^{L} Y_{LM}(x)^2 = 1 \]
Shell: set of \((2L+1)\) orbitals, some or some \(n\).

Filled Shell: when all \((2L+1)\) orbits are occupied.

\(\frac{1}{n^6}\) has meaning only within HF picture (but this is not so far from reality).

HF energy matrix elements in new basis:

\[ U_{\text{direct}} = \sum_{n', L'} \sum_{m'} \int d^3x \int d^3y \frac{1}{1^2} \frac{\left| U_{n' L'}(x) \right|^2 \left| U_{n' L'}(y) \right|^2 \left| U_{m' L'}(x) \right|^2 \left| U_{m' L'}(y) \right|^2}{\left| x^2 - y^2 \right|^2} \]

Suppose one of \(n, n'\) (say \(n'\)) come to filled shell.

Sum over \(m', L'\),

\[ U_{\text{direct}} \leq \left( \sum_{n, L} \right) \left( \sum_{n', L'} \right) \frac{(2L+1)}{4\pi} \int d^3x \int d^3y \frac{\left| U_{n' L'}(x) \right|^2 \left| U_{n' L'}(y) \right|^2 \left| U_{m' L'}(x) \right|^2 \left| U_{m' L'}(y) \right|^2}{\left| x^2 - y^2 \right|^2} \]

But then \(\int d^3y \frac{1}{1^2} \) is indep of direction of \(x\)

\Rightarrow orthogonality of \(Y_{L\alpha}\) \(\Rightarrow\) # occ orbitals in shell \(\leq 2L+1\).

\[ U_{\text{dir}} = \sum_{n, L} \sum_{n', L'} \frac{(2L+1)}{4\pi} \int d^3x \int d^3y \frac{\left| U_{n' L'}(x) \right|^2 \left| U_{n' L'}(y) \right|^2 \left| U_{m' L'}(x) \right|^2 \left| U_{m' L'}(y) \right|^2}{\left| x^2 - y^2 \right|^2} \]

Direct interaction between filled shell + par filled shell indep of which orbitals occupied in par filled Dcp only on near charge dens.
Exchange

\[ U^{\text{ex}} = \sum_{m=-\infty}^{\infty} \sum_{m'} \int d^3x \int d^3y \ \frac{U^*_{nl}(x) U_{n'l}(y) U^*_{m'l}(x) U_{m'l}(y)}{1x-y} \]

\[ x \leq \sum_{m''} y^*_{l'm''}(x) y_{l'm''}(y) y^*_{l'm''}(x) y_{l'm''}(x) = \frac{2L'+1}{4\pi} P_L(x-y) \]

\[ \sum_{m''} y^*_{l'm''}(x) y_{l'm''}(y) P_L(x-y) \]

- Everything in this eq is invariant under similitude rotations of \( x, y \) exc.

\[ \sum_{m} y^*_{lm}(x) y_{lm}(y) \Rightarrow \text{must pull out rotationally invariant part of this term} \]

\[ \sum_{m} y^*_{lm}(x) y_{lm}(y) \Rightarrow \text{same as if sum over all } m \]

\[ \sum_{m} y^*_{lm}(x) y_{lm}(y) \Rightarrow \text{mult by } \frac{1}{2L+1} \]

\[ U^{\text{ex}}_{\text{filled}} = \sum_{n} \sum_{l'} \frac{(2L'+1)M_l}{(4\pi)^2} \int d^3x \int d^3y \ \frac{U^*_{nl}(x) U_{n'l}(y) U^*_{m'l}(x) U_{m'l}(y)}{1x-y} \]

\[ x \leq \sum_{m''} y^*_{l'm''}(x) y_{l'm''}(y) P_L(x-y) P_L(x-y) \]

Summary: Int bet filled part filled shells indep. of everything but "sphericalized charge density" in each shell:

\[ \text{Can't give } L \text{ or } S \text{ dependence} \]
widely made assumption - useful for thinking purposes but not highly accurate.

Modification of filled shell wave functions due to interaction v/ port filled shell is negligible \( \Rightarrow \) int between port filled (d) + filled shells is linear in \# of d-electrons

\[
E_{\text{HF}}^{\text{Appr}} \left[ \text{Filled Shell}, N_d, l, s \right] = E_0 + N_d \cdot E_d + d-d \text{ int } \left[ l, s, n \right]
\]

\( E_d \) involves int v/ filled shells

Probably safer: assume also contribute to nonlinear dep. of \( E \) on \( N_d \) from these ints. Get by LDA, DFT or...

Now look at \( E_{\text{dd}} \) in detail. Dep on \( \delta N_d \),

+ on "configuration" (\( l, s \) values)

- Many states:
  - \( N_d = 1 \):
    - 10 states \([5p, 5l]\)
  - \( N_d = 2 \):
    - 30 triplet \([5x^{1/2}, x^3]\)
    - 15 singlet \(5 + 5x^{1/2}\)

For given \( N_d \). Classify states by total \( S \), total \( L \).

\( \langle H, L \rangle = \langle H, S \rangle = 0 \), write \( H \) in this basis as

near diagonal

2. Applied group theory: problem of Slater, Racah
Consider interactions within same shell:

$$U_{LL}^{\text{direct}} = 2 \sum_{m,m'} \int_0^\infty x^2 dx \int_0^\infty y^2 dy \left| U_L(x_1) \right|^2 \left| U_L(y_1) \right|^2 \times \int d^2 x_2 d^2 y \frac{\left| Y_{lm}(x_1) \right|^2 \left| Y_{lm}(y_1) \right|^2}{|x_1 - y_1|}$$

$$U_{LL}^{\text{exch}} = 2 \sum_{m,m'} \int_0^\infty x^2 dx \int_0^\infty y^2 dy \left| U_L(x_1) \right|^2 \left| U_L(y_1) \right|^2 \times \int d^2 x_2 d^2 y \frac{Y_{lm}^*(x_2) Y_{lm}(y_1) Y_{lm}(x_1) Y_{lm}^*(y_2)}{|x_1 - y_1|}$$

Note: radial parts same for both direct + exch.

' deal w/ same shell

Consider angular int. $x > y \Rightarrow \frac{1}{|x-y|} = \sum_K \frac{Y_{lm}^*(x) Y_{lm}(y)}{x^{K+1}} P_K(x,y) = \sum_K \frac{Y_{lm}^*(x) Y_{lm}(y)}{x^{K+1}} \sum_{m=-l}^l \frac{\delta_{m,-l}}{2K+1} \delta_{2K+l}$

⇒ direct: need term in $\left[ Y_{lm}^*(x) Y_{lm}(y) \right] Y_{Km'p}(x)$ which transforms as singlet under rot. of $x$

- what $K$ can I get to by adding $Y_l$ and adjust $z$?

Answer: 2L, 2L-2, 0

Exch: $Y_{lm}^*(x) Y_{lm}(y) Y_{Km'p}^*$ similar.
All Coulomb matrix elements need radial integrals

\[ F_0 \quad F_2 \quad F_4 \]

For p-shell

For d-shell

\[ F^L_x = 4 \int_0^\infty x^2 dx \int_0^\infty y^2 dy \frac{|U_L(x)|^2 |U_L(y)|^2}{x^{k+1}} \]

\[ = 4 \int_0^\infty x^4 dx \frac{|U_L(x)|^2}{x} \int_0^\infty \frac{dz}{z} U_L(2x) \]

Recall F has dimension of energy.
Recall: must use optimized radial wave functions.

* Slater defines: \( F_{\text{av}} \): energy of sphericalized charge dist: what you would get if you avg above expr. for \( E \) over all \( m \), \( m' \)

\( \text{"center of gravity of multiplet"} \)

For p: \( E_{\text{av}} = F_0 - \frac{2}{25} F_2 \)

\( \text{x \# of distinct pairs} \)

For d: \( E_{\text{av}} = F_0 - \frac{2}{63} F_2 - \frac{2}{63} F_4 \)

* Slater gives: energies for all configurations in terms of \( E_{\text{av}} + F \) 's.

You should think: \( E_{\text{av}} \): not so well known (int \( u \) filled shells etc). Rest of energy: effect of pairwise d-d interactions. \( F \) form, presence of pairs \( F_0, F_2, F_4 \) follows from group theory. Values: HF estimates.

Note empirical: higher energy states! energy est's less good. CI more imp't as \( \text{go up} \).
Note: Values of \( f_0 \)s depend on HF wave functions which depend on ionization state (or empirically depend on ionization state) HF estimates. Typically 20-50% above empirical estimates

Some examples:

Some #s: \( \text{Fe} \ [\text{HF}] \) \( 3p^6 3d^8 \) con R.g. \( F_0^{3d^3d} = 1.4 \text{ Ry} \)

\[ F_2 = 0.6 \text{ Ry} \]
\[ F_4 = 0.4 \text{ Ry} \]

RATIO: \( F_2/F_4 \approx 0.6 \# \), very small variation

Typical rule of thumb (will see indications later) \( F_0, \alpha, E_{au} \) strongly (factor of 2 or more) chased by solid state effects ("screening") \( F_2, F_4 \) rather (more precisely, multiplet splittings at fixed \( N \)) much less affected
Some examples (many more in Slater’s book)

Oxygen p-shells \[ 1s^2 2p^2 2p^{2p^N_i} \]

\( N_p = 1 \) \( l = \frac{3}{2} \) \( 9x \) (3 or 6, 3spw) \( \epsilon_p \)

\( N_p = 2 \)

\( 3p \) \( [L = 1, S = 1] \)

\[ E_{cv}^{(2)} - \frac{3}{25} F_2 \quad 9x \]

\( 'D \) \( [L = 2, S = 0] \)

\[ E_{cv}^{(3)} + \frac{3}{25} F_2 \quad 5x \]

\( 'S \) \( [L = 0, S = 0] \)

\[ E_{cv}^{(2)} + \frac{12}{25} F_1 \quad 1x \]

\( N_p = 3 \)

\( 4s \) \( [L = 0, S = \frac{3}{2}] \)

\[ E_{cv}^{(3)} - \frac{9}{25} F_2 \quad 4x \]

\( 2D \) \( [L = 2, S = \frac{1}{2}] \)

\[ E_{cv} \quad 1x \]

\( 2p \) \( [L = 1, S = \frac{1}{2}] \)

\[ E_{cv} + \frac{6}{25} F_2 \quad 6x \]

\[ \epsilon_p \quad \frac{3p}{N = 1} \quad \frac{2p}{N = 2} \quad \frac{3s}{N = 3} \]

Relation to simple notations

Hunds Coupling: \( N_p = 2 \) Triplet lowest: \( \frac{6}{25} F_2 \) to 1st singlet

\( N_p = 3 \) 3/2 lowest \( \frac{9}{25} F_2 \)

U: extra energy to change: 2 defects: cus or cf lowest
U: \[ E_{mp}^0 = 2 + E_{mp}^0 = 0 - 2E_{mp}^1 = 1 \]

\[ E_{av}^{(2)} = E_{av} - 2E_p \left( \frac{-3}{25} F_2 + \frac{3}{25} F_2 + \frac{12}{25} F_2 \right) \]

HF: \[ E_{av}^{(2)} = 2E_p + F_0 - \frac{2}{25} F_2 - \text{all } F_1's \approx \text{Ry/Severe} \]

Next point: hole picture: quantum numbers for removed electron from filled shell same as g's for adding to empty. If measure all energies from filled shell, formulas exactly same.

d electrons

\[ N_d = 1 \]
\[ ^2D \quad [L=2, S=\frac{1}{2}] \quad E_d' \]

\[ N_d = 2 \]
\[ ^3F \quad [L=3, S=1] \quad E_{av}^d - \frac{58}{441} F_2 + \frac{5}{441} F_4 \]

\[ ^3P \quad [L=1, S=1] \]
\[ E_{av}^{dav} + \frac{72}{441} F_2 - \frac{30}{441} F_4 \]

\[ ^1G \quad [L=4, S=0] \]
\[ E_{av}^{dav} + \frac{50}{441} F_2 + \frac{15}{441} F_4 \]

\[ ^1D \quad [L=2, S=0] \]
\[ E_{av}^{dav} + \frac{-13}{441} F_2 + \frac{50}{441} F_4 \]

\[ ^1S \quad [L=0, S=0] \]
\[ E_{av}^{dav} + \frac{140}{441} F_2 + \frac{140}{441} F_4 \]

\[ E_{av} = F_0 - \frac{2}{63} F_2 - \frac{2}{63} F_4 \]

Again Hund's coupling: Lowest \[ N_d = 2 \]: \[ S = 1 \quad L = 3 \]
Some #s

$^{46}Ti$: 3d$^n$

Empirical #

$E^e V$: 3.5, 1.6, 0.7 [Ry]

$F^2$: 0.45, 0.35 [Ry]

→ change of size of HF orbital

Multiplet en [eV]

$^3F$: 21, 22.2, 22.6, 22, 25

$^3P$: 21, 22.2, 22.6, 22.8, 25

$^3G$: 21, 22.2, 22.6, 22, 25

$^3D$: 21, 22.2, 22.6, 22, 25

$^3S$: 21, 22.2, 22.6, 22, 25

$^3P$: 21, 22.2, 22.6, 22, 25

$E_0$: not avail. $d^1, d^2, d^3 \Rightarrow U = 13.6 \text{eV} \approx 1 \text{Ry}$

$E_d \approx 2.8 \text{Ry}$


Hunds effects: probably not so important. $J_H: 1 \text{eV}$

This state is $L=3$ but ligand field will mix up $L$'s; $\Rightarrow$ effect probably smaller

Mn: empirical $E^e V$: not avail.

$d^5$

$F_2$: 15, 16, 17 [Ry]

Many States: mostly high spin

6s 6p 4F 4D 4P 4I 2H ... 2S

-5.24 -261/4 -0.03 -1.38, 1.8

$4F$ 4D

$\Rightarrow$ lowest spin flip energy: $-3 \text{eV}$

Note here are v. far from filled shell
Fundamental Question: how much of this multiplet stuff is important for behavior of actual solids

\[ \text{U}^\text{V}: \text{energy to change valence} \]
\[ \text{J}^\text{Hunds coupling - nature of low lying multiplets} \]
U: Fundamental definition: average of multi.
   part of energy dep. only on \( N \).

\[ E_{n+1} + E_{n-1} - 2E_n = \frac{(n+1)n - 2n(n-1) + (n-1)(n-2)}{2} \quad U = U \]

However, in most cases, multiplets are spread
over too wide a range \( \Delta \) center differences
not useful \( 3 \)

Typically \( U \approx 15 - 20 \text{ eV} \)
- Better to consider energy differences \( \Delta \)
  between low-lying multiplets. Typically smaller
- Better to do this case-by-case

J: I prefer: energy difference between
   lowest energy (max spn) next lowest
   (max - 1 spn).
Mn energy levels—Ag host

Energy levels for single Mn in Ag host.
S,D,...refer to orbital symmetry of many electron wave function; superscript numerals give value of \((2S_{\text{tot}}+1)\)
Free-ion \(F_2, F_4\) and adjusted \(U\)

**Key points:**
- High spin states strongly favored
- In solid environment \('U' not so big

From van der Marel, Westra, Sawatzky and Hillebrecht, PRB 31 1936 (1985).

Fig. 2
TABLE III. On-site Coulomb ($U$) and exchange ($J$) energies estimated using the constrained LDA method (Anisimov et al., 1991), compared with the empirical estimates for the Racah parameter $A$ and charge-transfer energy $\Delta$ (Zaanen and Sag-watzky, 1990). $U_{\text{eff}}$ is the splitting between the $d^{n-1}$ and $d^{n+1}$ high-spin states. Energies are in eV.

<table>
<thead>
<tr>
<th></th>
<th>$U$</th>
<th>$J$</th>
<th>$U_{\text{eff}}$</th>
<th>$A$</th>
<th>$\Delta$</th>
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</tbody>
</table>
U estimated from photemission experiments (Imada et al RMP)
Renormalization
Solid state effects:

1) Hybridization: electron in d orbital can go into other states on solid.

2) As seen in Anderson model, levels get width

3) Ambiguity in definition of d-levels
   [seen before in Hartree-Fock level unambiguous, in exact soln: many particle state]
   Here more serious: atom: definite quantum \#s \# not conserved

To define \# d electrons, various methods

Simplest: "atomic sphere approx"

\[
\begin{align*}
0 \quad O_Tm \quad 0 \\
\end{align*}
\]

\[
\text{Drew sphere, some radius, (half-way to next atom?)}
\]

Then within sphere evaluate e.g. \[
\left| \sum_{\text{levels}} \int \frac{\mathbf{k}}{2\pi} \frac{1}{Z_0} \psi_N(x) \psi_N(x') d^3x \right|^2
\]

Projected d choice

Ambiguities: radius of sphere
Potential: not sph \# sym (sometimes approx. as)

Difficult to vary choice by integer amounts
Typically: estimate "0" by putting making small variations
Specifically put, in sphere $\langle Y_{2n} \rangle$
\[
\text{chemical potential to force density variation - typically alternate from cell to cell (ch. neutral)}
\]
\[
\Rightarrow \text{work out } \frac{8E}{\delta n^2} \text{; get rid of } \frac{8\gamma}{\delta n} \quad U \delta n
\]
Interpret remainder as $U$. - Typ.

Note: includes "relaxation" - are finding lowest energy configuration. Different result if don't let surrounding relax. Typically: in $3d$ oxides: $U^{4+}$. Dev. metals: $U^{3+}$ few.

Big? - How fast is relaxation?
If it can happen as fast as $U^{-1}$, then is it a reasonable thing to do?