Lecture 11 — 10/16

(iii) size: $\langle r \rangle = \frac{1}{2}\left(3n^2 - l(l+1)\right) a$

(iv) $\Delta E = Z^2 \, Ry \left(\frac{1}{n^2} - \frac{1}{n'^2}\right)$

c) Angular momentum (What happens for $2e^-$? or for combination of orbital ang. mom. and spin?)

in general (any ang. mom): $\vec{J} = \vec{r} \times \vec{p}$

$\vec{J} \times \vec{J} = i\hbar \vec{J}$ ⊗

$$\left.\begin{aligned} \vec{J}^2 |j, m_j\rangle &= \hbar^2 j(j+1) |j, m_j\rangle \\ \hat{J}_z |j, m_j\rangle &= \hbar m_j |j, m_j\rangle \end{aligned}\right\} \otimes\otimes$$

⊗, ⊗⊗ are equivalent

$\Rightarrow \hat{J}_\pm |j, m_j\rangle = \hbar \sqrt{j(j+1) - m(m \pm 1)}\, |j, m_j \pm 1\rangle$

Addition: $\vec{J} = \vec{J}_1 + \vec{J}_2$

$[\vec{J}^2, \vec{J}_{1/2}^2] = [\vec{J}, \vec{J}_{1/2}^2] = 0$

$[\vec{J}^2, \vec{J}_{1/2}] \neq 0$

(because: $\vec{J}^2 = \vec{J}_1^2 + \vec{J}_2^2 + 2\vec{J}_1 \cdot \vec{J}_2$)

- Eigenstates (of coupled ang. mom. operators)

1) "uncoupled representation":

$|j_1, m_1, j_2, m_2\rangle$: good q. numbers (full desc. of system)

but not eigenstate of $\vec{J}^2$

2) "coupled representation"

$|j, m, j_1, j_2\rangle$ (also good q. nb.)

eigenstate of $\vec{J}^2, J_z, \vec{J}_1^2, \vec{J}_2^2$, but not of $\hat{J}_{1z}, \hat{J}_{2z}$

$\Rightarrow$ transformation?

$$|j,m,j_1,j_2\rangle = \sum_{m_1,m_2} |j_1,m_1,j_2,m_2\rangle \underbrace{\langle j_1,m_1,j_2,m_2|j,m,j_1,j_2\rangle}_{\circledast}$$

$$|j_1,m_1,j_2,m_2\rangle = \sum_{j,m} |j,m,j_1,j_2\rangle \underbrace{\langle j,m,j_1,j_2|j_1,m_1,j_2,m_2\rangle}_{\circledast}$$

$\circledast$: $\boxed{\text{"Clebsch-Gordan coefficient"}}$

only $\neq 0$ for $m_1+m_2=m$

$$|j_1-j_2| \leq j \leq |j_1+j_2|$$

$$\left(\sum_{j=|j_1-j_2|}^{|j_1+j_2|} (2j+1) = (2j_1+1)(2j_2+1) \right)$$

(later needed to calculate transition dipole elements)

- <u>Spin-orbit coupling</u>

$\vec{L}, \vec{S} \;\hat{=}$ magnetic moment

they interact!

$$H_{LS} = V_{LS}(r)\, \vec{L}\cdot\vec{S}$$

Spin $\vec{S}$: found via Stern-Gerlach, but is so far only postulated, <u>does not</u> follow from S. Eq!

$H = H_0 + H_{LS}$ does not commute with $\vec{L},\vec{S}$, but it commutes with $\vec{J} \equiv \vec{L}+\vec{S}$

$$\langle \vec{L}\cdot\vec{S} \rangle = \frac{1}{2}\langle J^2 - L^2 - S^2 \rangle$$

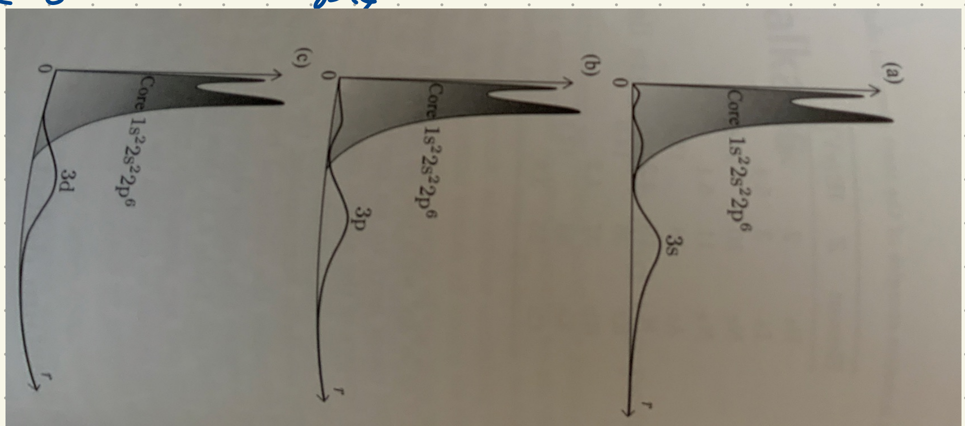
$$= \frac{\hbar^2}{2}\left(j(j+1) - l(l+1) - s(s+1)\right)$$

$$\overset{\text{single } e^-}{=} \frac{\hbar^2}{2} \begin{cases} l & \text{for } j = l+\frac{1}{2} \\ -(l+1) & \text{for } j = l-\frac{1}{2} \end{cases}$$

Quantum defect

Atoms with one outer-shell $\bar{e}$ (eg all alkali):
it is ok approximation to use same potential as for hydrogen (since effective potential same)

<u>But</u>: finite probability density <u>inside</u> inner shell. (see Foot pic)



$\Rightarrow$ short range potential changed!

$$V_{tot} = V_{coulomb,H} + V_{short-range}$$

$$\hookrightarrow \lim_{r \to \infty} V_{sr} \, r^2 \overset{!}{=} 0$$

$\Rightarrow$ energy values E_n follow same rules ($E_n \propto \frac{1}{n^2}$) but with different n:

$$E_n = - \frac{Z^2 \, Ry}{(n - \delta_l)^2}$$

"quantum defect"

		$l=0$	$l=1$	$l=2$	$l=3$
$n=2$,	Li	0.4	0.04	0	0
$n=3$	Na	1.35	0.85	0.01	0
$n=4$	K	2.19	1.71	0.25	0
$n=5$	Rb	3.13	2.66	1.34	0,01
$n=6$	Cs	4.06	3.58	2.46	0,02

(Calculational approx: "Central field approx": see Foot)

Rydberg Atoms

Def. Atoms with outer e^- excited into state with very high principal quantum number n.

Properties (guesses)

- high energy (i.e., very close to continuum limit)
- large orbits
- looks qualitatively like (large) H-atom (i.e., [nucleus + other e^-] $\ll$ orbit, i.e. look like nucleus
- large dipole $\Rightarrow$ high sensitivity to external fields, other Rydberg atoms, ...

Scaling (from Adams, Pritchard, Shaffer, J. Phys B 53, 012002 (2020))

Property	Quantity	Scaling
Energy levels	E_n	n^{-2}
Level spacing	ΔE_n	n^{-3}
Radius	$\langle r \rangle$	n^2
Transition dipole moment ground to Rydberg states	$\lvert\langle n\ell\rvert - er\lvert g\rangle\rvert$	$n^{-3/2}$
Radiative lifetime	τ	n^3
Transition dipole moment for adjacent Rydberg states	$\lvert\langle n\ell\rvert - er\lvert n\ell'\rangle\rvert$	n^2
Resonant dipole–dipole interaction coefficient	C_3	n^4
polarisability	α	n^7
van der Waals interaction coefficient	C_6	n^{11}

Why? $E_n \propto -\frac{1}{n^2}$

- Scaling of $\langle r^s \rangle$ with n? with l?

  <u>$s>0$:</u> large r dominates behavior; largely independent of l (nodal structure in r dominates $\langle \ldots \rangle$-integral)

  <u>$s<0$:</u> $r \to 0$ dominates; l small more important (because large l has low probability density near $r=0$).

- in general: n replaced by $n^* = n - \delta$ (quantum defect)

$\Rightarrow$ with Bohr radius $r = \frac{n^2 \hbar^2}{4\pi\epsilon_0 e^2 \mu}$ $\Rightarrow \langle r \rangle \propto n^2$

$\Rightarrow \langle r^s \rangle \propto n^{2s}$ for $s>0$

$\Rightarrow \langle \frac{1}{r} \rangle \propto E_n \propto n^{-2}$ $\quad (s=-1)$

$\Rightarrow \langle r^s \rangle \propto n^{-3}$ $\quad (s<-1)$ $\quad$ why?

$\Rightarrow$ Energy: $\propto n^{-2}$

$\Delta E \propto n^{-3}$

dipole moment $\propto n^2$ $\quad$ $(\langle f | er | i \rangle \propto \underbrace{\langle r \rangle}_{\propto n^2} \underbrace{\langle l_f | \cos\vartheta | l_i \rangle}_{\text{indep of } n}$

cross section $\sigma \propto \langle r^2 \rangle \propto n^4$

lifetime: $\tau \propto n^3, n^5$ $\quad$ $(\gamma \propto \omega^3 r_{if}^2$

Ryd $\to$ Ryd $n \to n'$ $\quad n^{-9}$ $\quad n^2 \to n^{-5}$ $\quad$ (circular)

Ryd $\to$ ground $\quad \sim n^0$ $\quad l=0, \propto n^{-3/2} \to n^3$ (to g.s.)

polarizability $\alpha \propto n^7$ $\quad$ (Stark shift $\Delta E \propto \alpha E^2$

$$\Delta E \text{ (pert. th)} = \sum \frac{|\langle nlm | er | n'l'm' \rangle|^2}{E_{nl} - E_{n'l'}}$$

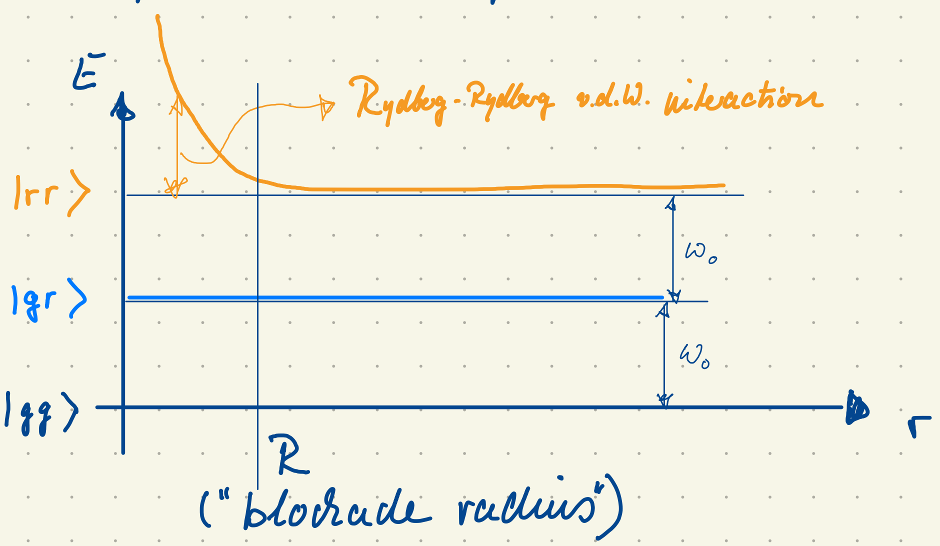
$\underbrace{n^2 \qquad \frac{1}{n^3}}_{n^7}$

v.d. Waals interaction $\propto n^{11}$ $\quad$ $\frac{\alpha_A \cdot \alpha_B}{r^6} = \frac{n^7 \cdot n^7}{n^3} = n^{11}$

Applications

- very strong interactions,
  use for: controllable interactive ensembles
- high sensitivity to el. DC fields
  use for: sensing
- sensitivity for μw, THz rad.
  use for: detecting
- Highlight: $\boxed{\text{Rydberg blockade}}$

<u>Idea:</u> very strong interaction between Rydberg atoms shifts transition out of resonance.



(distance between Rydberg atoms)

Normally: for two Rydberg atoms, one photon of frequency ω_0 excites one atom into $|r\rangle$, a second photon leads to $|rr\rangle$.

For small r: $\frac{1}{r^6}$-dependent van-der Waals interaction pushes the $|gr\rangle \to |rr\rangle$ transition out of resonance.

$\Rightarrow$ within a radius R, only one atom can maximally be excited into the Rydberg state, more excitations are blocked.

R is typically defined as the radius where the interaction strength equals the linewidth of the excitation transition.

A few review articles:

Saffman, Walker, Mølmer, RMP <u>82</u>, 23123 (2010)

Adams, Pritchard, Shaffer, J. Phys. B (AMO) <u>53</u>, 012002 (2020)

Dunning, Killian, www.scientia.global/rydberg-atoms-giants-of-the-atomic-world/

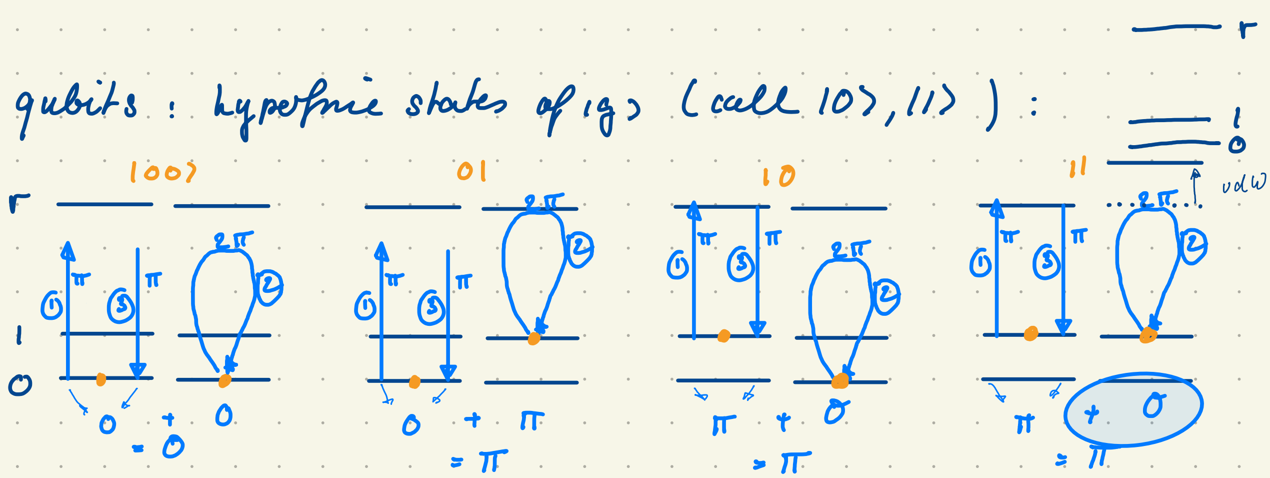
Gate using Rydberg blockade:

phase gate: $$\begin{array}{c|cccc} & 00 & 01 & 10 & 11 \\ \hline 00 & & & & \\ 01 & & & & \\ 10 & & & & \\ 11 & & & & \end{array} \quad \underbrace{\begin{pmatrix} a & & & \\ & b & & 0 \\ & 0 & c & \\ & & & d \end{pmatrix}}_{U}$$

U is a nonlinear gate if $|a| = |b| = |c| = |d| = 1$ and normalize to $a = 1$

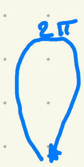
$\Rightarrow \arg b + \arg c \neq \arg d$

qubits: hyperfine states of $|g\rangle$ (call $|0\rangle, |1\rangle$):



$$U = \begin{pmatrix} 1 & & & \\ & -1 & & \\ & & -1 & \\ & & & -1 \end{pmatrix}$$

: π-pulse



: 2π pulse

One 2π-pulse on a transition (or a combination of 2 π-pulses) gives an overall shift of π. The same pulse <u>not</u> on a transition does nothing.