RYDBERG ATOMS

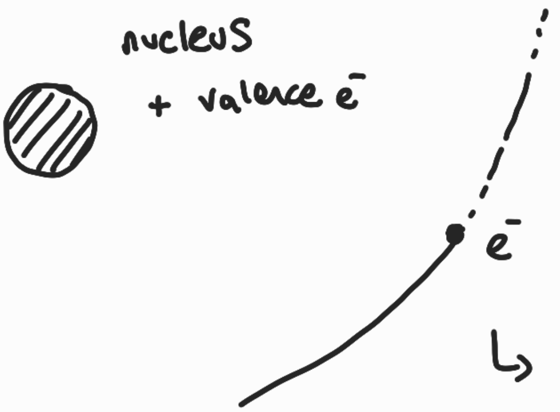
Single Atom as quantum information carrier

I. Introduction

1) Hydrogen-like atoms

Consider 1 e^- all other e^- are "frozen"

(which is ok for highly excited state)



e^- promoted to highly excited state

↳ bound by Coulomb potential $V(r) = \frac{-e^2}{4\pi\varepsilon_0 r}$

It has rotational invariance.

Schrödinger Equation :

$$\left[-\frac{\hbar^2}{2m_e} \Delta + V(r) \right] \Psi_e = E \Psi_e$$

$$[\hat{L}^2, \hat{H}] = 0 \quad , \quad [\hat{L}_z, \hat{H}] = 0$$

So $\Psi(r) = \frac{U(r)}{r} Y_\ell^m(\vartheta,\varphi)$

$|\Psi\rangle = |n\ell m\rangle$

$\hat{L}^2 |\Psi\rangle = \hbar^2 \ell(\ell+1) |\Psi\rangle$

$\hat{L}_z |\Psi\rangle = \hbar m |\Psi\rangle$, $m \in \{-\ell, \dots, \ell\}$

Radial part:

$$-\frac{\hbar^2}{2m_e}\frac{d^2}{dr^2} u_{n\ell}(r) + \underbrace{\left(V(r) + \frac{\hbar^2(\ell+1)\ell}{2mr^2}\right)}_{V_{eff}(r)} u_{n\ell}(r) = E_{n\ell}\, u_{n\ell}(r)$$

Spectrum: $E_n = -\frac{Ry}{n^2}$, independent of ℓ $\quad Ry = \underbrace{\frac{1}{2}\frac{me^4}{\hbar^2}}_{Ry_\infty = 13{,}6\ eV}\left(\frac{M}{M+m_e}\right)$

Remarks: . For real atoms $E_{n\ell} = \frac{-Ry}{(n-\mu_\ell)^2}$ $\quad \mu_\ell$: quantum defect

. Length scale $\quad a_0 = \frac{4\pi\epsilon_0\hbar^2}{m_e e^2}$ Bohr radius $\quad a_0 = 5{,}3 \times 10^{-11} m$

. Rydberg atom: atom with an e^- in state $n \geq 20\text{-}100$

2) Scaling

- "size" of an atom (with n increasing)

$$\left\langle \frac{1}{r} \right\rangle \sim \frac{4\pi\epsilon_0}{-e^2} \langle V(r) \rangle$$

Virial theorem: $\langle V(r) \rangle \propto E_n$

$$\Rightarrow \left\langle \frac{1}{r} \right\rangle \sim \frac{1}{n^2 a_0} \quad \Rightarrow \text{" size"} \sim n^2$$

$\rightarrow$ principal quantum number

★ Dipole moment :

$$\langle n\ell m | \hat{\vec{d}} | n'\ell' m \rangle \qquad n' \sim n \,, \quad \ell' = \ell + 1$$

$$\sim e a_0 n^2$$

$$\left(\Psi_{n\ell m}(r) \sim r^{n-1} e^{-r/a_0} \right)$$

II. Atomic Interactions

1) Van der Walls Potential

Neutral atom, polarizable

Dipole - dipole interaction:

$$U(r) = \frac{1}{4\pi\epsilon_0 r^3} \left(\hat{\vec{d}}_A \cdot \hat{\vec{d}}_B - 3 (\vec{u} \cdot \hat{\vec{d}}_A)(\vec{u} \cdot \hat{\vec{d}}_B) \right)$$

$\rightarrow$ from classical electrodynamics

For quantum problem: $\mathcal{H}_{rel} = \mathrm{Sp}\{|\vec{k}\rangle, \vec{k} \in \mathbb{R}^3\}$

relative

$\mathcal{H}_A = \mathrm{Sp}\{|nlm\rangle, \dots\}$ $\quad \mathcal{H}_B = \dots$

Atom

Born-Oppenheimer Approximation: e^- are fast

Perturbation Theory:

- 1^{st} order $\quad \langle n_A l_A m_A : n_B l_B m_B | \hat{U} | n_A l_A m_A : n_B l_B m_B \rangle = 0$

  since $\langle d_A \rangle_{nlm} = 0$

- 2^{nd} order $\quad \Delta E^{(2)} = \sum_{\nu, \nu'} \frac{|\langle n_A l_A m_A : n_B l_B m_B | \hat{U} | \nu, \nu' \rangle|^2}{E_{n_A l_A n_B l_B} - E_{\nu \nu'}} \neq 0$

Scaling: $\quad \Delta E^{(2)}(r) = -\frac{C_6}{r^6}$ $\quad C_6$ is a number depending on the "details".

- $\langle n_A | \hat{\vec{d}}_A | \nu \rangle \sim n^2$, same for B

- $U \sim n^4$

- $\langle U \rangle^2 \sim n^8$

$$E_{n_A n_B} - E_{pp'} = \delta E$$

derivative

Since $E \sim \frac{1}{n^2} \Rightarrow \delta E \sim \frac{1}{n^3}$

$$\Rightarrow C_6 \sim n^{11}$$

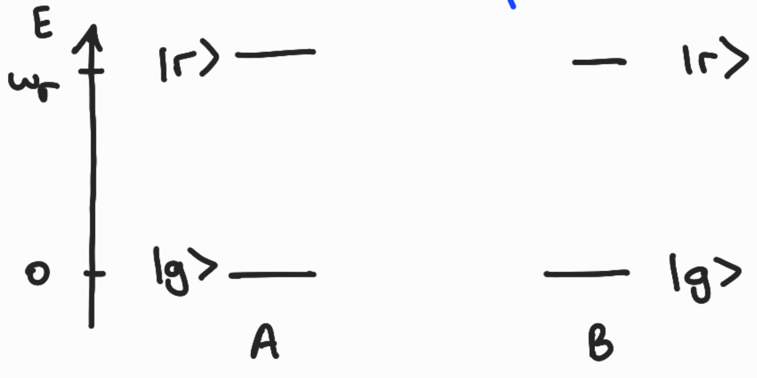
Van der Waals potential: $V_{vdw}(r) = -\frac{C_6}{r^6} \sim n^{11}$

Remark:

Van der Walls force exists between any pair of polarizable objects

There are situation for which first order is non-zero $\frac{C_3}{r^3}$ interaction

2) Two-Atom Spectrum



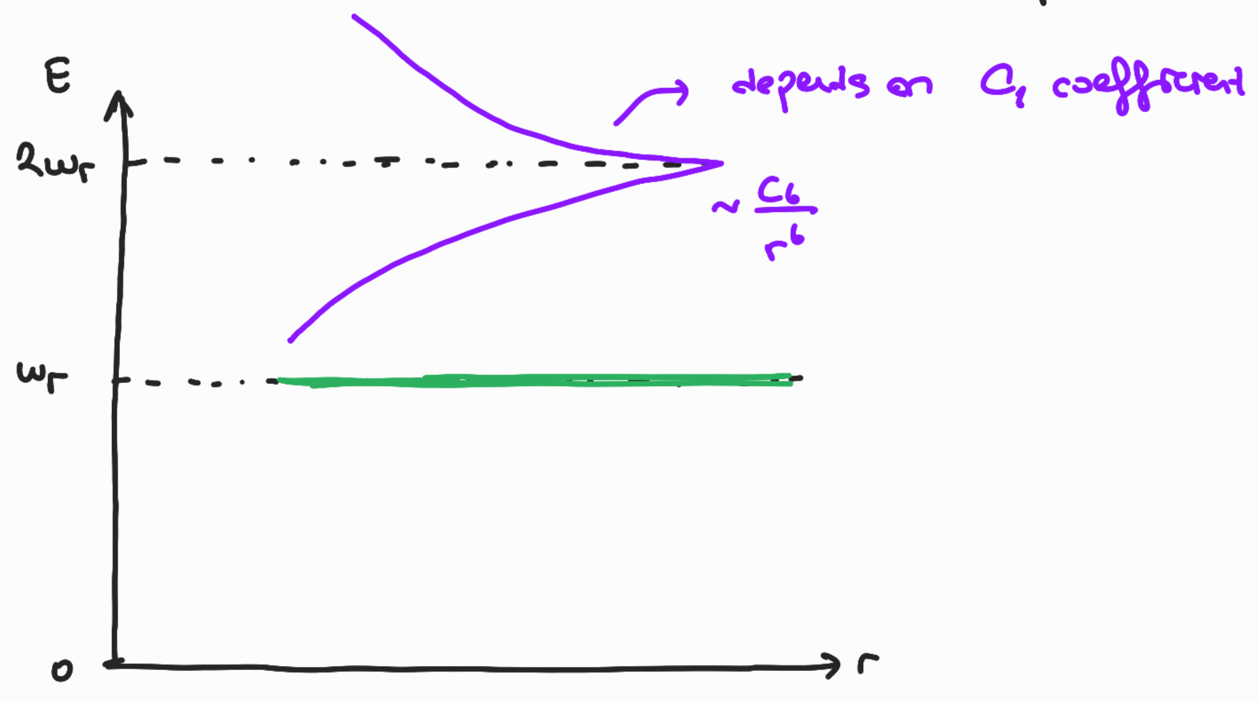
. Very weak interaction between $|g\rangle$ and $|g\rangle$

& btw $|r\rangle$ and $|g\rangle$?

Hilbert space:

$$Sp\{|gg\rangle, |gr\rangle, |rg\rangle, |rr\rangle\}$$

$$\hat{H}_{at} = \omega_r |gr\rangle\langle gr| + \omega_r |rg\rangle\langle rg| + 2\omega_r |rr\rangle\langle rr| - \frac{C_6}{r^6} |rr\rangle\langle rr|$$



3) Rydberg Blockade

We are driving hamiltonian $|g\rangle \longrightarrow |r\rangle$

$$\hat{H} = \hat{H}_{at} + \frac{\Omega}{2}\Big(\underbrace{|r\rangle\langle g| \otimes \hat{\mathbb{I}}}_{\text{atom A}}\, e^{-i\omega_L t} + \hat{\mathbb{I}} \otimes \underbrace{|r\rangle\langle g|}_{\text{Atom B}} e^{-i\omega_L t} + h.c.\Big)$$

for $\omega_L = \omega_r$, move to the rotating frame:

$$|r\rangle \longrightarrow |r\rangle e^{i\omega_L t}$$

$$|r,r\rangle \longrightarrow |r,r\rangle e^{+2i\omega_L t}$$

$$\hat{H} = -\frac{C_6}{r^6} |rr\rangle\langle rr| + \frac{\Omega}{2}\Big(|r\rangle\langle g| \otimes \hat{\mathbb{I}} + \hat{\mathbb{I}} \otimes |r\rangle\langle g| + hc\Big)$$

• For $C_6 = 0$: Dicke States description

Drive will induce coherent spin states

• For $\frac{C_6}{r^6} \gg \Omega$: $\hat{\mathbb{1}} = |r\rangle\langle r| + |g\rangle\langle g|$

$$\hat{H} = -\frac{C_6}{r^6}|rr\rangle\langle rr| + \frac{\Omega}{2}\Big(|rg\rangle\langle gg| + |rr\rangle\langle gr| + h.c.$$

$$|gr\rangle\langle gg| + |rr\rangle\langle rg| + h.c.\Big)$$

Move to rotating frame:

$$\hat{U} = e^{-i\frac{C_6}{r^6}|rr\rangle\langle rr| t}$$

$$|rr\rangle \longrightarrow e^{-i\frac{C_6}{r^6}t}|rr\rangle$$

Rotating wave approximation:

$\frac{C_6}{r^6}$ is a large frequency wr to the other scales.

$$\hat{H}_{RWA} = \frac{\Omega}{2}\Big(|rg\rangle\langle gg| + |gr\rangle\langle gg| + h.c.\Big)$$

Using RWA: we went from 4d Hilbert space to 3d $\mathcal{H}$ space

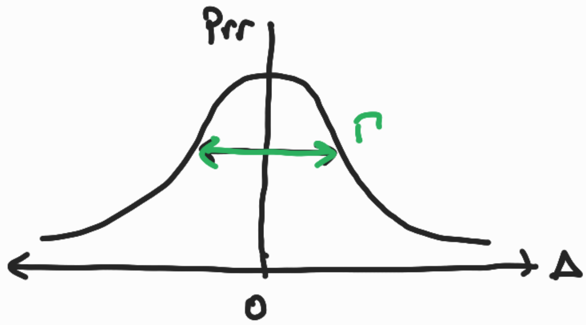
$|rr\rangle$ has dropped.

"Rydberg Blockade"

How far can 2 atoms be for blockade to take place?

$|rg\rangle \longrightarrow |rr\rangle$: 2-level system

$\Rightarrow$ Optical Bloch Equations



$\Delta = (E_{rr} - E_{rg}) - \omega_L$
laser

$\Delta = \omega_r - \frac{C_6}{r^6} - \omega_r$

$= -\frac{C_6}{r^6}$

If $\frac{C_6}{r^6} \gg \Gamma, \Omega$

Blockade happens

$$r_b = \left(\frac{C_6}{\Gamma}\right)^{1/6}$$

(blockade) radius

In practise $r_b \sim 10\mu m$

III. Applications

$$\hat{H} = \frac{\Omega}{2}\left(|rg\rangle\langle gg| + |gr\rangle\langle gr| + hc\right)$$

$$= \frac{\Omega\sqrt{2}}{2}\left(|\psi^+\rangle\langle gg| + hc \right) \qquad |\psi^+\rangle = \frac{1}{\sqrt{2}}\left(|gr\rangle + |rg\rangle \right)$$

$(g=0,\ r=1)$

Bell State

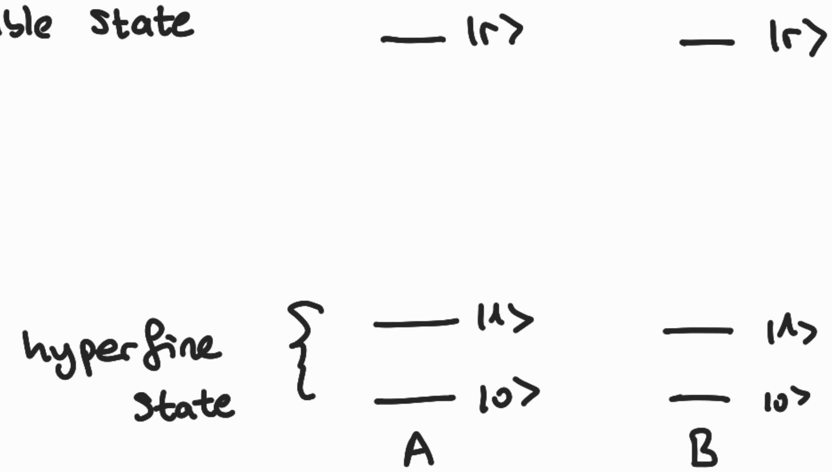
After $1/2$ Rabi cycle: Bell State

Remark . $\sqrt{2} \leftrightarrow$ superradiance

. For two atoms: Bell / Dicke state $j=1$ are identical. But no way to create Dicke state from $|gg\rangle$ using coherent drive

1) 2 qubit gate

$|r\rangle$ is not a stable state



. 2 atoms at distance $\ll r_b$

. drive selectively transitions btw $|1\rangle \longrightarrow |r\rangle$ without affecting $|0\rangle$
$\downarrow$
A or B

Remark: For a 2-level system 2π rotations $\Leftrightarrow$ $\times(-1)$

$$\hat{U}_x(\theta) = e^{-i\frac{\theta}{2}\hat{\sigma}_x} = \cos\frac{\theta}{2}\,\mathbb{I} - i\sin\frac{\theta}{2}\,\hat{\sigma}_x$$

for $\theta = 2\pi$: $\hat{U}_x(2\pi) = -\hat{\mathbb{I}}$

$\hookrightarrow$ important for CNOT

Pulse sequence:

1. π-rotation of qubit A: $|1\rangle_A \longrightarrow |r\rangle_A$
2. 2π-rotation of qubit B: $|1\rangle_B \longrightarrow -|1\rangle_B$
3. π rotation of A : $|r\rangle_A \rightarrow -|1\rangle_A$

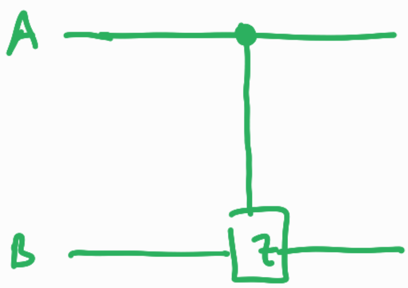
Truth Table:

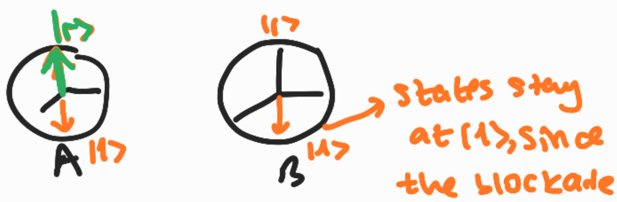
$|00\rangle \longrightarrow |00\rangle$

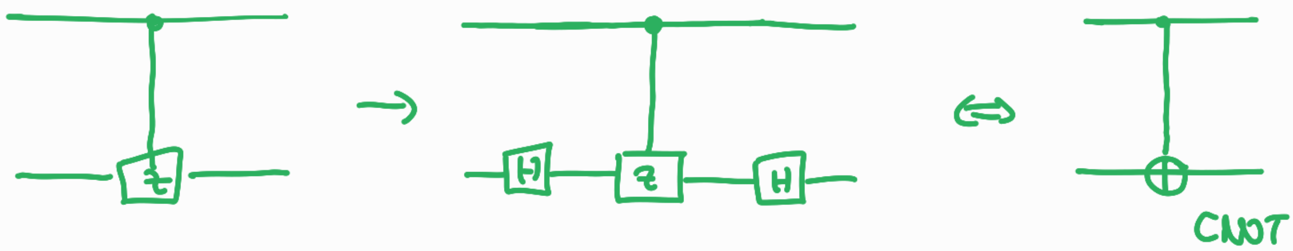
$|10\rangle \longrightarrow -|10\rangle$

$|01\rangle \longrightarrow -|01\rangle$

$|11\rangle \longrightarrow -|11\rangle$







2) Quantum Simulation

$|g\rangle |r\rangle$ describe 2 level system $\Leftrightarrow$ spin 1/2 particle in $\vec{B}$ field

- Rydberg atom, driven by laser $|g\rangle \longrightarrow |r\rangle$

Single atom: $\hat{H} = \omega_r |r\rangle\langle r| + \frac{\Omega}{2}\left(|r\rangle\langle g| e^{-i\omega_L t} + h.c.\right)$

(Rotating frame) $= \delta \hat{\sigma}_z + \frac{\Omega}{2}\hat{\sigma}_x$ + constant

Atomic ensemble: $\hat{H} = \sum_i \delta \hat{\sigma}_z^{\,i} + \frac{\Omega}{2}\hat{\sigma}_x(i)$

$- \sum_{i<j} \frac{C_6}{R_{ij}^6} \hat{n}_i \cdot \hat{n}_j$

$\hat{n}_i = I \otimes I \otimes \cdots \otimes |r\rangle\langle r| \otimes \cdots \otimes I$

$= \frac{1}{2}\left(\mathbb{I} + \sigma_z^{(i)}\right)^i$

↓

Rewritten as

$$\hat{H} = \sum_i (\delta + B_i)\,\hat{\sigma}_z^{(i)} + \frac{\Omega}{2}\hat{\sigma}_x^{(i)} + \sum_{i<j} J_{ij}\,\hat{\sigma}_z^{(i)}\hat{\sigma}_z^{(j)}$$

$$B_i = \sum_j -\frac{C_6}{R_{ij}^6}$$

"Ising Model"
with transverse field

Properties:

- Paramagnetic Phase

- Fero/antiferromagnetic phase