# L4 Quantum information and computing (QIC)

# Lecture 16: Rydberg atoms (DVC2.2)

January 6, 2023

Aims of Lecture 16: To understand how to make atom interact between atoms allow us to create entanglement.

#### **Introduction:**

In QIC.15 we learnt how to drive single-qubit rotations using stimulated Raman transitions. So we can tick off the single-qubit gates part of DVC2. But to make a quantum computer we need two-qubit gates as well. We need two-qubit gates to access all the  $2^N$  states, mostly entangled states that will give us quantum advantage. To realise two-qubit gates and/or entanglement we need interactions but atoms are neutral and do not interact, or atleast, only interact very weakly. To solve this problem we use laser excitation to highly-excited state where the electron is very far from the nucleus. These states are commonly known as **Rydberg states**. In our energy level map, Rydberg state appear very close the ionisation limit, the dashed line in Fig. 1. As we shall see Rydberg atom can have very strong interactions.

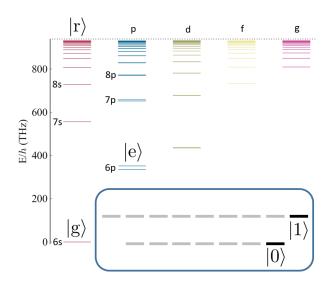


Figure 1: The energy level of the Cs atom. The magnetic sub-levels within the ground state are shown inset. A Cs atom quantum computer uses hyperfine ground states,  $|0\rangle$  and  $|1\rangle$  for the computational basis, an excited state  $|e\rangle$  for initialisation, single-qubit rotations and read-out, and a highly-excited Rydberg state  $|r\rangle$  for two-qubit gates.

**Rydberg atoms** To find the size and energy of atoms as a function of the principal quantum number n, we use the Bohr quantization rule

$$mv_nr_n=n\hbar$$
,

where the electron speed,  $v_n$  is given by equating the centripetal force and the Coulomb attraction,

$$\frac{mv_n^2}{r_n} = \frac{e^2}{(4\pi\epsilon_0)r_n^2} ,$$

i.e.  $v_n^2=e^2/[m(4\pi\epsilon_0)r_n]$ . Substituting into the quantization formula all squared gives  $me^2/[(4\pi\epsilon_0)]r_n=n^2\hbar^2$  and therefore

$$r_n = n^2 \frac{\hbar^2}{me^2/(4\pi\epsilon_0)} = n^2 a_0 .$$

where  $a_0$  is the Bohr radius. This shows that the **size of** a **Rydberg atom** scales as  $n^2$ . An n=100 Rydberg atom is about a micron across—avery big atom! As dipole moments are given by charge times distance, the dipole moment also scales as  $n^2$ . The lifetime is inversely proportional to the dipole moment between the Rydberg state and the ground state  $\langle \mathbf{g} | -er | \mathbf{r} \rangle$ 

The energy of state n (using the virial theorem equal to one half of the potential energy) is given by

$$E_n = -\frac{e^2}{2(4\pi\epsilon_0)r_n} = -\frac{R_{\rm H}}{n^2} ,$$

where  $R_{\rm H}$  is known as the **Rydberg constant**. This is known as the Rydberg formula. A similar formula applies to all atoms with one electron in a Rydberg state.<sup>1</sup> It follows that the spacing between Rydberg states scales a

$$E_n = -\frac{R_{\infty}}{(n - \delta_{n,\ell})^2} .$$

<sup>&</sup>lt;sup>1</sup>Only we need to adjust the Rydberg constant and there is an energy shift due to the interaction between the electron and the core (nucleus plus other electrons). This shift is included via a quantum defect,  $\delta_{n,\ell}$ , so we have

## Interactions

The giant size of Rydberg atoms leads to giant electric dipole moments (for transitions between a Rydberg state  $|\mathbf{r}\rangle$  and another Rydberg state  $|\mathbf{r}'\rangle$ ), and strong van der Waals interactions. To estimate the van der Waals shift we consider a pair of atom in a Rydberg state  $|\mathbf{r}\rangle$ . Each atom experiences the electric field created by the other dipole which has the form  $\mathcal{E}_{\rm d} = \mathcal{D}_0^2/(4\pi\epsilon_0 R^3)$ , where R is the distance between the atoms, and  $\mathcal{D}_0 = \langle \mathbf{r}' | \mathbf{d} | \mathbf{r} \rangle$  is the dipole matrix element associated with a transition between Rydberg states  $|\mathbf{r}\rangle$  and  $|\mathbf{r}'\rangle$ . In the pair basis  $\{|\mathbf{rr}\rangle, |\mathbf{r}'\mathbf{r}'\rangle\}$  the dipole-dipole interaction,  $\mathcal{H}_{\rm dd} = -\mathbf{d} \cdot \boldsymbol{\mathcal{E}}$ , is

$$\mathcal{H}_{\mathrm{dd}} = \hbar \left( egin{array}{cc} 0 & V \ V & \Delta_{\mathrm{pair}} \end{array} 
ight) \, ,$$

where

$$V = \frac{\mathcal{D}_0^2/\hbar}{4\pi\epsilon_0 R^3} \; ,$$

and  $\hbar\Delta_{\rm pair}$  is the energy difference between the pair states  $|{\bf r}'\rangle$  and  $|{\bf r}\rangle$ . For  $|\Delta_{\rm pair}|\gg V$ , the frequency shift of  $|{\bf r},{\bf r}\rangle$  is

$$V_{
m vdW} = \frac{V^2}{\Delta_{
m pair}} \ .$$

This is known as the **van der Waals** interaction. Note it can be either positive or negative depending on whether the state  $|\mathbf{r}'\rangle$  is below or above  $|\mathbf{r}\rangle$ . As V is proportional to  $1/R^3$ , the van der Waals interaction is proportional to  $1/R^6$ .

As V is proportional to the dipole matrix element squared and hence the principal quantum  $n^4$ , and the energy difference  $\Delta_{\text{pair}}$  scales as  $1/n^3$ , the van Waals interaction scales as  $n^{11}$ , and the interaction between two atoms in a high-excited Rydberg state is at least 12 orders of magnitude larger than between two ground state atoms. The van der Waals shift can be either positive or negative depending on whether the nearest Rydberg states have lower or higher energy.

## **Summary:**

What do you need to be able to do?

1. Understand the scaling properties of Rydberg atoms as a function of their principal quantum number, n. This include the size, dipole moment, energy level spacing, and van der Waals interaction strength.