# Building Blocks for Quantum Computing Part III

### "Quantum Mechanics and Atomic Physics " Primer

Patrick Dreher CSC801 – Seminar on Quantum Computing Spring 2018

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### Goal Is To Understand The Principles And Operation of the Trapped Ion Quantum Computer (TIQC)

- Building Blocks for Quantum Computing Part I
- Building Blocks for Quantum Computing Part II
- Building Blocks for Quantum Computing Part III Quantum Mechanics Primer
- Building Blocks for Quantum Computing
   Design and Construction of the TIQC Part IV
- Building Blocks for Quantum Computing Operation of the TIQC – Part V

# What Components are Included in the Experimental Apparatus of an Ion Trap QC



NIST Ion Trap Apparatus

# **Key Components in a TIQC**

- To discern how a Trapped Ion Quantum Computer (TIQC) works need to identify key components
  - Atoms and Materials
  - Electromagnetic fields
  - Lasers
  - Experimental samples are deposited in extremely low temperature experimental chambers (cryostats)
- Examine these components one at a time to understand their role in a TIQC

### "Quantum Mechanics Primer" for Atoms and Materials

### Start by Selecting a Material for the TIQC

- Experimentalists select specific elements because
  - Unique atomic properties when interacting with electromagnetic waves
  - Various properties of the atom can be mapped to the operations of a qubit
- Questions
  - What is the selection criteria for specific materials?
  - How and why do they work in a TIQC?

### **Properties of All Materials**

- All materials are atoms that are made of protons, neutrons and electrons
- Protons and neutrons form the nucleus of the atom
- Electrons surrounding nucleus reside in atom's energy levels
- Electrons occupy energy shells surrounding the nucleus
- Inner shells will fill first
- All types of atoms are globally classified and organized in a Periodic Table of the Elements



# **Periodic Table of Elements**

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	
1	1 <sup>1</sup> H Hydrogen 1.00794	Atomic # Symbol Name Atomic Mass	С	Solid		[		Metals	;	]	Nonmet	als						2 <sup>2</sup> He Helium 4.002802	К
2	3 Li Lithium 6.941	4 2 Be Beryllium 9.012182	H. H	g Liquid Gas		Alkali me	Alkaline earth me	Lanthanc	netals	Poor me	0 Other nonmeta	Noble ga	5 23 B Boron 10.811	6 24 C Carbon 12.0107	7 25 N Nitrogen 14.0067	8 <sup>2</sup> 0 Oxygen 15.9994	9 <sup>2</sup> / <sub>7</sub> F Fluorine 18.9984032	10 % Ne Neon 20.1797	ĸ
3	11 <b>Na</b> <sup>Sodium</sup> 22.98976928	12 2 Mg Magnesium 24.3050	R	<b>f</b> Unknov	vn	tals	tals	Actinoids	3 -	tals	<u></u>	ises	13 28 Al Aluminium 28.9815388	14 <sup>2</sup> Si Silicon 28.0855	15 <sup>2</sup> <b>P</b> Phosphorus 30.973762	16 28 Sulfur 32.085	17 28 CI Chlorine 35.453	18 <sup>2</sup> Ar Argon 39.948	K L M
4	19 K Potassium 39.0983	20 28 Ca 28 Calcium 40.078	21 <sup>2</sup> <b>Sc</b> Scandium 44.955912	22 <b>Ti</b> <sup>11</sup> Titanium 47.887	23 23 28 V 11 Vanadium 50.9415	24 28 Cr 13 Chromium 51.9961	25 Mn Manganese 54.938045	<sup>2</sup> <sup>3</sup> <sup>13</sup> <sup>13</sup> <sup>13</sup> <sup>13</sup> <sup>13</sup> <sup>13</sup> <sup>13</sup>	<sup>2</sup> <sup>14</sup> <sup>14</sup> <sup>2</sup> <b>Co</b> <sup>1</sup> <sup>1</sup> <sup>1</sup> <sup>1</sup> <sup>1</sup> <sup>1</sup> <sup>1</sup> <sup>1</sup>	28 Ni Nickel 58.6934	29 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 3 2 9 1 2 3 2 9 1 2 9 1 2 9 1 2 9 1 2 9 1 2 9 1 1 2 9 1 1 1 2 9 1 1 1 2 1 1 1 1	30 28 <b>Zn</b> 2 Zino 65.38	81 8 <b>Ga</b> 3 Ballium 9.723	32 <sup>2</sup> <b>Ge</b> <sup>18</sup> Germanium 72.84	33 2 <b>As</b> Arsenic 74.92160	34 28 Se 8 Selenium 78.96	35 28 Br <sup>18</sup> Bromine 79.904	36 <sup>2</sup> Kr <sup>18</sup> Krypton 83.798	K L M N
5	37 <b>Rb</b> <sup>Rubidium</sup> 85.4678	38 28 Sr 82 Strontium 87.62	39 2 Y 18 Yttrium 88.90585	40 <b>Zr</b> <sup>2</sup> irconium 91.224	41 28 Nb 12 Niobium 92.90838	42 28 Mo 18 Molybdenum 95.96	43 <b>Tc</b> Technetium (97.9072)	<sup>2</sup> <sup>8</sup> <sup>18</sup> <sup>14</sup> <sup>14</sup> <sup>14</sup> <sup>14</sup> <sup>14</sup> <sup>14</sup> <sup>14</sup> <sup>14</sup>	<sup>2</sup> <sup>18</sup> <sup>18</sup> <sup>18</sup> <sup>18</sup> <sup>18</sup> <sup>18</sup> <sup>10</sup> <sup>10</sup> <sup>10</sup> <sup>10</sup> <sup>10</sup> <sup>10</sup> <sup>10</sup> <sup>10</sup>	46 Palladium 108.42	<sup>2</sup> 8 <b>Ag</b> <sup>1</sup> <sup>1</sup> <sup>1</sup> <sup>1</sup> <sup>1</sup> <sup>1</sup> <sup>1</sup> <sup>1</sup> <sup>1</sup> <sup>1</sup>	48 28 Cd 18 Cadmium 112.411	19 2 18 <b>n</b> 18 13 14ium 14.818	50 28 <b>Sn</b> 18 Tin 118.710	51 28 <b>Sb</b> 18 Antimony 121.780	52 28 <b>Te</b> 18 Tellurium 127.60	53 2 8 18 18 18 18 7 Iodine 128.90447	54 28 Xe 18 Xenon 131.293	K L M NO
6	55 <b>CS</b> Caesium 132.9054519	56 28 Ba 18 Barium 2	57–71	72 <b>Hf</b> <sup>11</sup> Hafnium 178.49	73 28 <b>Ta</b> 180.94788	74 28 W 18 Tungsten 2 183.84	75 <b>Re</b> Rhenium 188.207	<sup>2</sup> <sup>18</sup> <sup>18</sup> <sup>22</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup>	<sup>2</sup> <sup>18</sup> <sup>12</sup> <sup>14</sup> <sup>1</sup> <sup>11</sup> <sup>11</sup> <sup>12</sup> <sup>11</sup> <sup>11</sup> <sup>13</sup> <sup>14</sup> <sup>11</sup> <sup>11</sup> <sup>11</sup> <sup>12</sup> <sup>12</sup> <sup>11</sup> <sup>11</sup> <sup>12</sup> <sup>12</sup>	78 <b>Pt</b> Platinum 195.084	<sup>2</sup> <sup>8</sup> <sup>8</sup> <sup>7</sup> <sup>1</sup> <sup>1</sup> <sup>1</sup> <sup>1</sup> <sup>1</sup> <sup>1</sup> <sup>1</sup> <sup>1</sup> <sup>1</sup> <sup>1</sup>	80 28 Hg 18 Mercury 2 200.59	81 2 <b>TI</b> 32 hallium 3 04.3833	82 2 <b>Pb</b> 32 Lead 4 207.2	83 2 Bi 18 Bismuth 208.98040	84 2 <b>Po</b> Polonium (208.9824)	85 28 At 32 Astatine 7 (209.9871)	86 2 <b>Rn</b> 32 Radon (222.0176)	KLMNOP
7	87 2 Fr 18 Francium 1 (223)	88 2 Ra 18 Radium 22 (226)	89–103	104 <b>Rf</b> Rutherfordium 1 (281)	2 105 2 100 2 100 2 100 2 100 2 100 2 100 2 100 2 100 2 100 2 100 2 100	106 28 Sg 322 Seaborgium 12 (268) 22	107 Bh Bohrium (284)	108 18 32 32 32 4 Hassium (277)	2 8 109 12 12 14 2 14 2 14 2 14 2 109 11 1 33 33 109 11 33 11 33 11 11 33 11 11 11 33 11 11	2 110 Ds Darmstadtium (271)	<sup>2</sup> <sup>8</sup> <sup>8</sup> <sup>8</sup> <sup>8</sup> <sup>8</sup> <sup>8</sup> <sup>8</sup> <sup>8</sup> <sup>10</sup> <sup>10</sup> <sup>10</sup> <sup>10</sup> <sup>10</sup> <sup>10</sup> <sup>10</sup> <sup>10</sup>	Uub 32 Ununbium 2 (285)	113 Uut Ununtrium (284) 18 18 32 32 32 18 32 32 33 18 32 32 32 33 33 33 34 35 35 35 35 35 35 35 35 35 35	114 2 Uuq 32 Ununquadium 18 (289)	115 2 Ununpentium 18 (288) 22	116 <b>Uuh</b> Ununhexium (292)	117 Uus Unurseptum	118 <b>Uuo</b> Ununoctium (294) <sup>2</sup> 8 18 18 18 18 18 18 18 18 18	KLZNORG
	For elements with no stable isotopes, the mass number of the isotope with the longest half-life is in parentheses.																		
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	Dto	bla		57 La Lanthanum 138.90547	58 <b>Ce</b> Cerium 140.116	59 28 Pr 21 Praseodymium 2 140.90765	60 <b>Nd</b> Neodymium 144.242	2 2 2 2 2 2 2 2 2 2 2 2 2 2	62 18 23 23 5 23 2 5 23 5 23 5 20 20 20 20 20 20 20 20 20 20	63 <b>Eu</b> <sup>2</sup> <sup>2</sup> <sup>2</sup> <sup>2</sup> <sup>2</sup> <sup>2</sup> <sup>2</sup> <sup>2</sup>	64 64 63 64 64 64 74 74 74 74 74 74 74 74 74 74 74 74 74	65 28 <b>Tb</b> 27 Terbium 158.92535	66 28 <b>Dy</b> 28 182.500	67 2 Ho 29 Holmium 184.93032	68 28 Er 300 Erbium 2 167.259	69 <b>Tm</b> <sup>1</sup> Thulium 168.93421	70 <b>Yb</b> Ytterbium 173.054	71 2 Lu <sup>18</sup> Lutetium 2 174.9888	
		com		89	90 <sup>2</sup>	91 <sup>2</sup> <b>P</b> 2 <sup>16</sup>	92	<sup>2</sup> 93	<sup>2</sup> 94	95 Am	<sup>2</sup> 96	97 <sup>2</sup> BL <sup>16</sup>	98 <sup>2</sup> Cf <sup>16</sup>	99 <sup>2</sup> 5 5 <sup>16</sup>	100 <sup>2</sup> 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5	101 3	102 á	103 <sup>2</sup> I r <sup>18</sup>	

Fm

Fermium

(257)

No

(259)

Nobelium

Lr

(262)

Lawrencium

32 31

Md

Mendelevium

32 30

Actinium (227)

Th

Thorium 232.03808

Pa

Protactinium 231.03588

U

Uranium 238.02891

Np

Neptunium (237)

Pu

Plutonium (244)

Cm

Curium (247)

Am

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Americium

Bk

(247)

Berkelium

32

32 27 8

## **Bound States of Each Element**

- Each element in the Periodic Table has protons (and neutrons) in a nucleus and an equal number of electrons in bound states surrounding that nucleus
- There are different energy levels (n = 1, 2, 3, ...) that have bound states labelled as S, P, D, F, ...
- The electrons fill these bound states in a specific order
  - S state takes 2 electrons
  - P state takes 6 electrons
  - D state takes 10 electrons

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### **Order of Filling of Shells**



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# **Picking an Element for a TIQC**

- Choose Calcium in the 2<sup>nd</sup> column of the periodic table
- Calcium (Ca) has atomic number 20 (20 protons in the nucleus and 20 electrons filled in distinct energy bound state shells surrounding the nucleus)
- Interactions mainly occur among electrons in the partially filled outer shells
- Examine the atomic properties of Ca

### Examine the Atomic Structure of a Calcium Atom



### Order of Electron Filling of Energy Levels in Calcium Atom

# Electron Configuration Chart s holds up to 2 p holds up to 6 d holds up to 10 20 Calcium 40.08 $1s^{2}2s^{2}2p^{6}3s^{2}3p^{6}4s^{2}$

### **Electromagnetic Fields**

# **Electromagnetic Fields**

- Electromagnetic fields
  - Carry energy and angular momentum
  - Interact with electrons in atoms
- Key properties of atoms and electromagnetic fields
- Bound state electrons in an atom will absorb and emit discrete quantities of energy and units of angular momentum
- Electromagnetic fields are a primary source that transfers energy and angular momentum to electrons in the atom

### **Propagation of Electromagnetic Fields**



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## Transferring Energy to/from Bound State Electrons in an Atom

- The amount of energy that an electron absorbs/emits to change from an initial state to a different state is determined by
  - Difference between the two bound state energy levels
  - The initial and final angular momentum state (S, P, D, F,)
- The total angular momentum of the electron is determined by the combination of both the electron's orbital angular momentum and an "internal" angular momentum called "spin"

# Transferring Energy to/from Bound State Electrons in a Material

- By selecting a specific frequency of electromagnetic radiation it transfers energy and discrete units of angular momentum into an electron
- Results in an electron transitioning from an initial state to a different state
- There are specific "quantum mechanics" rules constraining transitions between energy levels based on the transition energy and change in angular momentum
- Rules are based on an electron's total angular momentum J (sum of orbital angular momentum (L) and internal spin angular momentum (S))
- Rules summarized as "Selection Rules"

### **Selection Rules for Atomic Spectra**

Electric dipole (allowed)		Magnetic dipole (forbidden)	Electric quadrupole (forbidden)			
(1) $\Delta J = 0, \pm 1$ (0 $\pm 0$ ) (2) $\Delta M = 0, \pm 1$ (3) Parity change (4) One electron ju $\Delta l = \pm 1$ For L - S court	Rigorous	$\Delta J = 0, \pm 1$ (0 \operatorname 0) $\Delta M = 0, \pm 1$ No parity change No electron jump $\Delta l = 0$ $\Delta n = 0$	$\Delta J = 0, \pm 1, \pm 2$ (0 \operatornameq 0, \frac{1}{2} \operatornameq \frac{1}{2}, 0 \operatornameq 1) \Delta M = 0, \pm 1, \pm 2 No parity change One or no electron jump \Delta l = 0, \pm 2			
(5) $\Delta S = 0$ (6) $\Delta L = 0, \pm 1$ (0 $\leftrightarrow 0$ )	, in B	$\Delta S = 0$ $\Delta L = 0$	$\Delta S = 0$ $\Delta L = 0, \pm 1, \pm 2$ $(0 \leftrightarrow 0, 0 \leftrightarrow 1)$			

### **Energy Levels and Transitions in Materials**

- Electrons can change energy states by transitioning among different quantized energy levels
- Electrons absorb and emit discrete quantities of energy and angular momentum when undergoing these transitions



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### Focus on the Atomic Spectra of Calcium



### Lasers

## **Electromagnetic Radiation Properties**

• Light is composed of many electromagnetic fields of many different energies (frequencies)



**Incoherent Light** 

 Need light with properties of coherence (light with specific frequency and common phase)



**Coherent Light** 

### Need a Focused Source of Energy - Lasers -

- It would be far more efficient to "dial-up" a specific energy difference that will cause the electron to transition (resonate) between two different energy levels
- Requires a coherent light source tuned to a specific frequency



# Lasers in the Experimental Apparatus

- Electromagnetic radiation from a laser will interact with the electronic structure of these particular atoms
- Laser can
  - Produce electromagnetic radiation across a spectrum of frequencies from infrared through ultraviolet
  - Be tuned to specific electron transition energies
- By varying the polarization, phase, wavelength, and duration of the laser light pulse the behavior of the electron can be controlled
- From a QC perspective this effectively created rotations and transformations of the qubit states

### **Calcium Atom Spectra**



### Consider the States Of <sup>40</sup>Ca Just Below And Above The Fully Filled Shells



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# Several Types of <sup>40</sup>Ca Energy Level Transitions That Can be Identified



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## Low Temperature Experimental Apparatus

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### **IBM Q Cryostat**



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### Requirement for Low Temperature Environment for the Experiment

- At room temperature the electrons are subject to many types of thermal fluctuations
- Above the filled electron shells, there are many unfilled bound states to which the electron can transition (unwanted volunteers)
- Want to suppress this "thermal jitter" so that the transitions between bound and excited states in the <sup>40</sup>Ca atom is minimized

### Minimize The Atomic Transitions in a Material by Cooling the Experimental Apparatus To Almost "Absolute Zero" Temperature



### Cool the Apparatus to Limit the Size of the Hilbert Space Available to the Qubit



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# Removing Unwanted Excited States to Prepare the Ion to Initially Only be in the S<sub>1/2</sub> Ground State

- Depopulate the P<sub>1/2</sub> ←→
   D<sub>3/2</sub> transition that can contaminate the D ←→ S long lived state for a qubit
- Also need to de-populate the D<sub>5/2</sub> state
- Need 2 new lasers (854 nm and 866 nm) to pump electrons to the  $P_{1/2}$  and  $P_{3/2}$  states that can then drain to the  $S_{1/2}$  ground state



# **Building a Long Lived Ion Qubit State**

- Now use another laser tuned to the resonant wavelength of (729 nm) to force an excited state population into the D<sub>5/2</sub> state |e> from the S<sub>1/2</sub> ground state |g>
- From laws of QM this is a forbidden transition and so the excited state will be long lived (~1 sec) compared to the lifetime of an allowed transition (~ 1 nanosecond) → stable qubit
- Now have constructed a long-lived stable qubit



# Toward The Construction of a Trapped Ion Quantum Computer

# **Goal of an Experimental TIQC**

- Goal is to construct an experimental apparatus that can
  - 1. Take 1 qubit inputs and produce outputs that reflect the properties of 1 qubit gates
  - 2. Take 2 qubit inputs and produce outputs that reflect the properties of 2 qubit gates
- Demonstrating an experimental apparatus that satisfies goals 1. and 2. above will form the basis for a universal quantum computer
- This process of building and operating a TIQC universal quantum computer will be described in detail in Lectures IV and V

### Last Slide

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