#### **OCHA-PP-381**

## Introductory Lecture on Quantum Computer

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#### Abstract

This is an introductory lecture, prepared for an undergraduate course of the schooling "Reading of Original Paper" at the Open University of Japan (OUJ), in the summer semester from June 6 to 27 in 2024. The purpose of the lecture is mainly to read and understand the Feynman's original paper, "Quantum Mechanical Computers (1986) [1]. As a supplement, some recent developments in the implementation of Quantum Computer are surveyed.

## 1 Lecture 1: Introduction of Feynman's paper (1986)

In the first lecture, we read the introduction of the paper [1] with the help of the description of Logic Gate in Wikipedia, and discuss on it.

#### 1.1 Prerequisite to understand the introduction

Feynman started with Bennett's claim (1979) that the dissipation caused by the quantum computation is essentially zero. Bennett asked Feynman to examine the validity of his result.

Usually the dissipation occurs by the *irreversible processes* where entropy S increases, by generating the heat Q,

$$dQ = TdS. \tag{1.1}$$

Feynman claims that the primitive elements of quantum computation are *reversible processes*, so that there is no thermodynamical loss, but the entropy represents the complexity of the system, or the amount of information contained in the system. It is Boltzmann who connects the entropy with an amount of the information, being identified with the existence probability W of the system,

$$S = k_B \ln W, \tag{1.2}$$

where  $k_B$  is the Boltzmann constant  $\approx 1[\text{eV}]/10^4[\text{K}]$ .

Usually information is given by an array of *binary numbers*, that of 0 or 1, such as 00110101. A single digit called a *bit*, consists of 0 or 1, so the minimum number of information

is 2, or the probability  $W \propto 2$ , and hence, the minimum energy loss associated with the change of single bit information, yields

$$\Delta Q = T\Delta S = k_B T\Delta(\ln W) = (k_B T)\ln 2. \tag{1.3}$$

This is the result by Bennet, guaranteed by Feynman.

The usual computer uses macroscopic materials such as wires, transistors and so on, so that the dissipation appeared per a bit is quite large,  $\Delta Q = 10^{10} k_B T$ . Compared to this, the energy loss of quantum computer is essentially zero, providing a dream machine at least theoretically without considering the realistic implementations.

#### 1.2 Primitive elements, or Logic Gates

Primitive elements of computation in [1] mean *Logic Gates*. We can learn symbols and truth tables for the logic gates, such as NOT, AND, OR, NAND, NOR, XOR, and XNOR from Wikipedia "Logic Gates" [2].



Figure 1: Logic Gate 1 from Wikipedia

Figure 2: Logic Gate 2 from Wikipedia

# 2 Lecture 2: From MOSFET to logic circuit for adder in Feynman's Sec.2

#### 2.1 Transistor circuit

In Fig. 2 of Feynman, we can find the electronic transistor circuits for "NOT" and "NAND" gates.

In this Figure, MOSFET transistor is used, one in "NOT" gate and two in "NAND" gate. *MOSFET* means Metal-Oxide-Semiconductor Field-Effect Transistor.

As shown in Figure 3, Feynman instructs how to symbolize MOSFET and Bipolar transistors as well as NOT Gate. The name of the terminals differs; for MOSFET they are Gate, Drain and Source, while for Bipolar they are Base, Collector and Emitter. The present IC (integrated circuit) uses MOSFET.<sup>1</sup>



Figure 3: Transistors; left: MOSFET, middle: Fig.2 of Feynman, and right: Bipolar

MOSFET plays the role of switch. If the enough voltage is applied to G (ON state, or Q=Yes), then a current flows from D to S. If the voltage is not enough (OFF or Q=NO), no current flows. Depending on Q =YES or NO, the voltage at Q' is V (defined as Q' = NO) or the smaller value 0 (defined as Q' =YES). Then, we have the "NOT" gate.

Similarly for "NAND" gate, only when two inputs a and b of Feynman are both ON ( $Q_1$  and  $Q_2$  are both YES in our case), the current flows and Q'=NO. Otherwise, the outputs are all YES. This gives the "NAND" gate.

At present, the resistance in Fig.2 of Feynman (and our Figure 3) is replaced by a p-MOSFET. Two types, positive (p-) and negative (n-) MOSFETs act conversely, since p-type and n-type semiconductors in their inner-structures are interchanged.

Look at the inner structure of n-MOSFET depicted in Figure 4. Here, we find three elements of the name, Metal, Oxide, and Semiconductor.

As is well-known, n-type semiconductor is Silicon (Si, atomic number Z = 14) doped with As (arsenic) having atomic number Z = 33. Si has four electrons in the 3rd shell, and becomes stable when four *covalent bond* are formed with extra four electrons supplied from outside. As has five electrons in the forth shell, so after forming four covalent bonds with Si, one electron remains, giving n-type semiconductor. On the other hand, if B (Boron) is doped (with Z=5), it has three electrons in the second shell, so one electron per B is missing to

<sup>&</sup>lt;sup>1</sup>The author owes largely to Akitoshi Nishimura who explained him the mechanism of circuit and MOS-FET, by showing Figure 3.



Figure 4: Inner structure of n-MOSFET

complete the four covalent bonds with Si. Thus, B-doped Si, gives the p-type semiconductor, which has an incomplete bond or a positive hole, with the same number of B atoms.

Even if the voltage acts between D and S, the n-type semiconductors are disconnected by the presence of the p-type semiconductor, so that no current flows between D and S.

The metal and semiconductor having SiO<sub>2</sub> in between, behaves like a "capacitor". Therefore, if the voltage is applied at G, the negative charges are invited to gather at the interface of SiO<sub>2</sub> and p-type semiconductor. As far as the voltage at G is small, or the electric field for the "capacitor" is small, then nothing happens, since all the electrons are trapped by the covalent bonds or holes. However, if the voltage  $V_G$  exceeds a certain threshold value  $V_{th}$ , then electrons in Source (n-type) start to flow into the thin layer under the SiO<sub>2</sub>/p-type Si interface, forming the "channel" to flow electrons from Source to Drain. Thus, we have understood why this device is called "field-effect transistor". The effect is caused by the strong electric field. This is as if p-type semiconductor becomes n-type one, and hence it is called the "inversion" occurs. Then, the gap between two n-type semiconductors are connected with an array of electrons, and the electric current flows from Drain to Source, induced by the voltage +V at Drain. This is why MOSFET plays the role of switch.

#### 2.2 Universality of the logic gates

Feynman stated that only one logic gate (universal gate) is enough to replicate all logic circuits. We can choose NAND or NOR as the universal gate, and use it repeatedly. This property was found by Charles Sanders Peirce in 1880-1881. See [2] for the details.

#### 2.3 Three reversible primitives

We will go to Sec.2 of Feynman, where "Computation with a Reversible Machine" is discussed.

Reversible machine was considered by T. Toffoli in 1981-1982.

Looking at the truth tables, NOT is reversible, that is, from the outputs a', the inputs a can be reproduced. However, other operations are not. For example, AND  $(a, b) \rightarrow c$ , is not reversible, since a single output c = 0 comes from three inputs (a, b) = (0, 0), (0, 1), (1, 0). Therefore, to obtain reversal elements, the number of bits should be increased to 2-bits or 3-bits.

A 2-bit example is "CONTROLLED NOT" (CNOT), and 3-bit one is "CONTROLLED CONTROLLED NOT" (CCNOT).

Look at Fig. 3 and Table 1 of Feynman, where the notation and truth table of CNOT is given as well as those of CCNOT, FAN OUT and EXCHANGE.

The CNOT is given by  $(a, b) \rightarrow (a', b')$ . The first bit a or a' is a controller with a = a'; if a = 0, b' = b, while if a = 1, b' = 1 - b as NOT operation.

Similarly, 3-bit CCNOT is defined with two controllers a and b; only if both controllers are 1, c' = 1 - c. Otherwise (can be expressed as ab = 0), c' = c.

The truth tables for them show that they are reversible.

For CNOT Feynman stated that  $b' = a + b \pmod{2}$  holds, but the expression b' = a+b-2ab is more useful. It can be used to repeat CNOT three times to form "EXCHANGE". FAN OUT is defined by CNOT for b = 0, since it gives a' = b' = a. FAN OUT means a single-bit number a spreads out (or duplicated) to two-bit ones (a, a).

#### 2.4 Logic circuit for adder

In Fig. 4 and 5, Feynman explained how to perform adder (addition operation).

1) Fig. 4 shows the sum of two numbers a and b. The first digit of the sum is b', and the second digit c' is prepared for the carry to appear. Namely,

$$b'(\text{SUM}) = a + b - 2ab, \ c'(\text{CARRY}) = ab.$$
(2.1)

"Carry" means the movement of the number at the lower digit to the upper digit (such as  $01 + 01 = 02 \rightarrow 10$ ). That is, if a = b = 1 then the sum becomes a + b = 2, which implies c' = 0, d' = 1. Therefore, we need to specify, in addition to SUM=0 (the first digit), the CARRY=1 of the second digit.

The first operation in Fig.4 is CCNOT, giving the CARRY c' = ab, while the second operation is CNOT, yielding b' = a + b - 2ab, the (SUM). Then, we understand that the logic gates in Fig.4 reproduce adder of two numbers correctly.

2) Fig.5 gives the sum of three numbers a + b + c. The first two operations in Fig.5 are identical to Fig.4, which generates the sum of two numbers a + b. Namely, we have s' = (1 - a)b + a(1 - b) = a + b - 2ab (SUM of a + b) and d' = ab (CARRY of a + b).

Next we go to the third and the forth operations, which describe the sum of s' + c, where

$$c'' = \text{SUM of } (s'+c) = s'+c-2s'c = (a+b+c)-2(ab+bc+ca)+4abc, (2.2)$$

giving (SUM) of a + b + c.

As for d'', we have

$$d'' = s'c(1 - d') + (1 - s'c)d', \text{ by using}$$
(2.3)

$$s' = a + b - 2ab, \ d' = ab, \ \text{we have}$$

$$(2.4)$$

$$d'' = (a+b-2ab)(1-2ab)c+ab,$$
(2.5)

which reads

$$d'' = \begin{cases} (a+b)c, \text{ if } ab = 0, \\ 1, \text{ if } ab = 1, \end{cases}$$
(2.6)

reproducing (CARRY) of a+b+c.

Now, the validity of Adder operations in Figure 5 (Fig.4 and 5 of Feynman) has been examined.



Figure 5: Feynman's Fig.4 and Fig.5, for adders

# 3 Lecture 3: Complete machine to quantum mechanical description of logic gate

#### 3.1 Complete machine

Feynman proceed further to his Fig.6. As is understood from the above adder operation, the output has more bits than the input; for the adder, the extra bits for carry are required. To be the machine reversible, in the initial stage, the input data plus extra bits with 0's have to be prepared, and in the final stage, the output data plus some garbages appear. The reversible correspondence is

• [Input data plus Extra bits with 0's]  $\Leftrightarrow$  •[Output data plus Garbages].

The machine does not want the garbage, so it is replaced by 0's.

Thus, we start with the extra qubits (containing 0's) in addition to the input qubits, operate the machine M as usual, and then we obtain the output data. At the same time, we

will devise to store the input data into the outer register by a succession of CNOT operations, since the input data will disappea during the operation M. Then, by inverse operation  $M^{\dagger}$  the machine will return to the starting point. This is pictured in Feynman's Fig.6.

In the machine, the garbage can be cleared to 0's.

Now, the real machine or the *complete machine* is obtained; it consists of the circuit M and its inverse  $M^{\dagger}$  as well as the Copy of the input and output, that is, the complete machine is build by  $(M, M^{\dagger}, \text{Copy})$ .

#### 3.2 Quantum mechanical computer

Next, we will read Sec.3 of Feynman, where "A Quantum Mechanical Computer" is discussed.

The logic operation is a transformation G of an initial n-digit binary  $(a, b, c, \cdots)$  to a final binary  $(a', b', c', \cdots)$ . We consider  $(a, b, c, \cdots)$  as a state vector in quantum mechanics of n two-level atoms,  $|\psi\rangle = |a\rangle|b\rangle|c\rangle\cdots$ . G can be a <u>unitary operator</u> or <u>unitary matrix</u>. If we choose the state vector of a single atom  $|a\rangle$  as

$$|a\rangle = c_1|1\rangle + c_2|0\rangle = \begin{pmatrix} c_1\\c_2 \end{pmatrix}, \text{ with } (c_1, c_2) = 1 \text{ or } 0, \tag{3.1}$$

we can introduce the creation  $a^{\dagger}$  and annihilation a operators as

$$\hat{a}^{\dagger} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad \hat{a} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}.$$
(3.2)

They satisfies,  $\{\hat{a}, \hat{a}\} = \{\hat{a}^{\dagger}, \hat{a}^{\dagger}\} = 0$ ,  $\{\hat{a}, \hat{a}^{\dagger}\} = 1$ . The notation  $\{\hat{A}, \hat{B}\} \equiv \hat{A}\hat{B} + \hat{B}\hat{A}$ , called anti-commutator. On the other hand, the commutator is defined by  $[\hat{A}, \hat{B}] \equiv \hat{A}\hat{B} - \hat{B}\hat{A}$ . (The anti-commutator appeared here represents the anti-commutation relations for "fermion", since a binary bit takes 0 or 1, as the occupation number of fermion is 0 or 1, not larger than two.)

The author has changed the notation with underline used by Feynman to that with hat, and the definition of creation and annihilation operators are reversed from [1].

Feynman uses the notation  $A_{ab\cdots, cd\cdots}$  for a logic operation where the former  $(ab\cdots)$  are controller bits, while the latter  $(cd\cdots)$  are target bits. Then, we have for NOT, CNOT, and CCNOT, as

$$A_a(\text{NOT}) = \hat{a} + \hat{a}^{\dagger}, \qquad (3.3)$$

$$A_{a,b}(\text{CNOT}) = (\hat{a}^{\dagger}\hat{a})(b+b^{\dagger}) + (\hat{a}\hat{a}^{\dagger}) = 1 + (\hat{a}^{\dagger}\hat{a})(b+b^{\dagger}-1), \qquad (3.4)$$

$$A_{ab,c}(\text{CCNOT}) = 1 + (\hat{a}^{\dagger}\hat{a})(\hat{b}^{\dagger}\hat{b})(\hat{c} + \hat{c}^{\dagger} - 1).$$
(3.5)

Feynman is very instructive, telling us how to read these formulae;  $(\hat{a}^{\dagger}\hat{a})$  and  $(\hat{a}\hat{a}^{\dagger})$ . They are operators to select  $|1\rangle$ (YES) and  $|0\rangle$ (NO), respectively, and we know that CNOT and CCNOT do not change state if one of the controllers is NO, while they act as NOT when all the control bits are YES. Following Feynman, we wish to understand mathematical formulae in terms of the spoken language.

In this lecture 3, the fundamentals of quantum mechanics in terms of Hamiltonian of 2X2 matrix was explained in detail, starting from how to calculate the product of matrices and explain what is the unitary matrix. Therefore, the time ran out before explaining the Hamiltonians for NOT, CNOT and CCNOT gates.

# 4 Lecture 4: From operator description of full adder to a way to run a program

#### 4.1 Operator to realize full adder

Since we have checked the validity of Figure 5, the operator M to perform the full adder operation can be written easily,

$$M = A_{a,b}A_{b,c}A_{bc,d}A_{a,b}A_{ab,d}.$$
(4.1)

Its inverse operation is done by its hermitian conjugate,  $M^{\dagger}$ , the inverse of the unitary operator. This reads

$$M^{\dagger} = A^{\dagger}_{ab,d} A^{\dagger}_{a,b} A^{\dagger}_{bc,d} A^{\dagger}_{b,c} A^{\dagger}_{a,b}.$$

$$\tag{4.2}$$

We already know that any operation can be constructed by successive application of a single universal operation such as CNOT or COR.

#### 4.2 Performing a given program

Usually computer calculation is performed line by line following a given program, in one direction from the upper line to the lower. The quantum mechanical reaction, however, accommodates always inverse reactions. This is a big problem. Feynman proposed how to carry out the program from the first line to the last, following line-ordering or time-ordering.

He introduces a program reading fermion (electron) at the *i*-th line of the program, with annihilation and creation operators  $\hat{q}_i$  and  $\hat{q}_i^{\dagger}$  of the fermion. The *i* runs from 0 to *k*. He considers *i* is a position of "cursor", so the fermion sites of i = 0 - (k+1) are called "program counter sites".

He introduces the Interaction Hamiltonian  $H_{RC}$ , between "Register" (R) made of n atoms and "Counter or Cursor" (C) made of k + 1 fermions. In the Register the calculations are done, while in Counter (or Cursor) the "program" is progressed by the counter fermions. That is,

$$H_{RC} = \sum_{i=0}^{k} \left( \hat{q}_{i+1}^{\dagger} A_i \hat{q}_i + \hat{q}_i^{\dagger} A_i^{\dagger} \hat{q}_{i+1} \right).$$
(4.3)

If the wave function of the Register is denoted as  $\psi(t)$ , the time development of the machine is given by

$$\psi(t) = M(t)\psi(0) = e^{-iH_{RC}t}\psi(0), \qquad (4.4)$$

$$M(t) = 1 - itH_{RC} + \frac{(-it)^2}{2!}(H_{RC})^2 + \frac{(-it)^3}{3!}(H_{RC})^3 + \cdots$$
(4.5)

At any time *i*, if the fermion field is excited only at a single site k = i,  $|q_i\rangle = |1\rangle$ , then the excitation  $|1\rangle$  moves straightforwardly (including the motion of back and forth in the middle) from  $|q_0\rangle$  to  $|q_k\rangle$ , and we obtain a realistic progression of computation,  $M(t) = \sum_{m \ge k+1} (-it)^m A_k A_{k-1} \cdots A_0 \propto A_k A_{k-1} \cdots A_0$ .

Although the backward motion of cursor produces  $A_i^{\dagger}$  which cancels  $A_i$  of the previous step, the same M remains finally as in the above.

This expectation is Yes for the classical (or ballistic) motion of the fermion, moving from i = 0 to i = k with the same momentum like a ball. However, the quantum motion of fermion is not a ball but a wave (packet), which interfere with another wave.

Even in quantum mechanics, if the system has an infinite size, a plain wave appears, which behaves like a classical ball. Since the size (number of lines of the program) is finite, however, a wave packet (a wave composed of various momenta) appears. Then, the estimation of the transition amplitude during a finite time interval t have to be estimated using wave packets,

$$T_{fi}(t) =_R \langle \psi_f(k) | \otimes_C \langle 0, \cdots, 1 | M(t) | \psi_i(0) \rangle_R \otimes | 1, 0 \cdots \rangle_C$$

$$(4.6)$$

which is not a easy task. So, Feynman considers to expand the Cursor sites to accommodate the plane waves for both initial and final Cursor states.

Therefore, how to carry out the quantum computation by reading a program, is an open problem. However, the hybrid system is allowed, in which the main body of calculation at register is quantum mechanical, while the other parts to read the program and to input and output of data are classical.

# 5 Lecture 5: Finish to read the Feynman's paper; by covering imperfection of quantum machine, the usage of switch and do loop and others

This section includes the important issues to build the actual quantum computers. Therefore, we will survey them roughly.

The next subsection discusses on "Imperfections of the machine and irreversible free energy loss".

#### 5.1 Imperfect motion of cursor and its energy loss

One origin of imperfections is the <u>back and forth motion</u> of the cursor, deviating from the expected ballistic motion of the cursor, moving straightforwardly from the first line of the program to the end line.

Feynman considered the motion of cursor as the motion of electron, which is not a free ballistic motion with a constant velocity  $v_B$ , but is perturbed by the trapped atoms of the Register. After a certain time has passed, it becomes a random motion with velocity  $v_B$ .

Assume the probability for a ballistic motion to a random motion, is p.

Here, let  $p_f$  be the probability to move forwardly from *i*-th line to (i + 1)-th line of the program, and  $p_b$  be the probability to move backwardly. Of course,  $p_f \gg p_b$  is assumed to hold.

The entropy loss for the cursor to move forwardly from i site to i + 1 site is

$$\Delta S/\text{step} = \ln p_f = \ln \frac{(p_f + p_b) + (p_f - p_b)}{2} = \ln \left(1 + \frac{p_f - p_b}{p_f + p_b}\right) - \ln 2 \tag{5.1}$$

$$\approx -\left(\frac{p_f - p_b}{p_f + p_b}\right) - \ln 2. \tag{5.2}$$

Denote total time (steps) actually spent be  $t_{actual}$ , and the minimum time for the ballistic case be  $t_{min}$ , then the loss of entropy per step reads

$$\Delta S/\text{step} = -\left(\frac{t_{min}}{t_{actual}}\right) = -\left(\frac{v_R}{v_B}\right).$$
(5.3)

In each step, the probability of converting the ballistic motion to the random motion is small equal to p, which Feynman called "coasting factor". Now the total entropy loss for the cursor movement is

$$\Delta S = -p\left(\frac{t_{min}}{t_{actual}}\right) = -p\left(\frac{v_R}{v_B}\right),\tag{5.4}$$

which gives the energy loss during the progression of program as

$$-\Delta E = k_B T \times p\left(\frac{t_{min}}{t_{actual}}\right) \ll k_B T.$$
(5.5)

Here, the probability is given by the inverse of the time spent. This result by Bennett was stated by Feynman.

He suggests the motion of quantum computer can be understood *as a heat engine*, that the reversible motion is possible, but it is when operated very slowly as a quasi-equilibrium process.

No energy loss arises from the uncertainty principle of the quantum computer.

However, due to the uncertainty principle  $\Delta E \Delta t \sim \hbar/2$ , the operation time  $\Delta t$  for a qubit is restricted by the energy gap  $\Delta E$  between two states  $|1\rangle$  and  $|0\rangle$  of a qubit. If the energy gap is 0.1 [eV], then the operation time is  $6 \times 10^{-15}$  [s], four orders of magnitude shorter than the operation time of the transistor.

Rather, a difficult problem is how to control the quantum mechanical interactions among atoms in the register, or between those of the register and the program processing counter site. This causes the decoherence in quantum mechanics, loosing the quantum information of qubits.

It is also pointed that the error correction codes (ECC) are very important. Many codes are known in the classical computation, but not much is known at that time in the quantum computation. After the Feynman's lecture, various ECCs are developed [9].

#### 5.2 Switch circuit in quantum computer

Similar to the MOSFET in the classical computer, the switch circuit can be built. See Fig.7 of Feynman in which the programing of the switch and its Hamiltonian are written. Its Hamiltonian reads

$$H_{\rm switch} = \hat{q}^{\dagger} \hat{c} \hat{p} + \hat{r}^{\dagger} \hat{c}^{\dagger} \hat{p} + \hat{p}^{\dagger} \hat{c}^{\dagger} \hat{q} + \hat{p}^{\dagger} \hat{c} \hat{r}.$$
(5.6)

Feynman uses the early alphabets,  $a, b, c, \cdots$  for the two-level atoms, while the later alphabets  $p, q, r, \cdots$  for the cursor fermions. The qubit of the atom c is called "flag"; depending on YES  $|1\rangle_c$  or NO  $|0\rangle_c$  of the flag at GATE, the operation is switched  $|p\rangle \rightarrow |q\rangle$  or  $|p\rangle \rightarrow |r\rangle$ , respectively.

Now, we go to Section 5 of Feynman.

#### 5.3 Simplification of quantum circuit by switches

This subsection is useful for the real implementation, since all the gates can be constructed with Switch and NOT gates.

For example, CNOT gate can be build with two Switches and one NOT. See Feynman's Fig.8.

Parts of the program can be M and N. Then, the conditional switch, depending on the state of the flag  $(|a\rangle)$ , can be constructed in Feynman's Fig.12.

Using this, we can build a complete machine in Feynman's Fig.13, called garbage clearer of  $(M, M^{\dagger}, \text{ Copy})$ ; by copying the result and recovering the machine to its original state having the input data.

"Do loops" are also constructed; Do M operations twice is given in Feynman's Fig.14, and Do M eight times in the same Fig.15.

Whenever the program is repeated, a new flag should be raised, since it is necessary to specify the number of times of the repetition in the quantum computation.

Feynman's Fig.16 of 3-bit increment counter, which the author felt difficult to understand, was clearly solved by a number of students who attended the lecture. It is necessary to know the most significant bit means the top digit c, when the number of count is  $2^2c + 2b + a$ .

As parts of the program, how subroutines are demonstrated is studied by Fredkin, Toffoli and Barnett in the paper to appear in 1986.

# 6 Lecture 6: Implementation of quantum computer by ultra-cold Rubidium atoms

Since we have finished to read Feynman's paper untill the last lecture, we are now allowed to survey the present status of the "implementation" of quantum computer, especially by using cold atoms of Rubidium (Rb).

#### 6.1 Making cold atoms and optical lattice by optical "tweezer"

We have to control two and three two-level atoms simultaneously, in order to operate CNOT and CCNOT gates, respectively.

To do this, a promising way is cooling atoms down to an extreme low temperature at  $\underline{\text{micro}}(10^{-6})$  or nano  $(10^{-9})$  Kelvin [K] to avoid the thermal agitations, and then we form a lattice of atoms. If a lattice point is occupied by a single two-level atom, it plays the role of a single qubit, and if using two atoms, 2 qubits are obtained, and so on. Here, "qubit" means "quantum-bit". The qubits located on such lattice points should be controlled so that they may form a certain logical circuit, properly connecting a number of logic gates. How to control the logical circuits is a big problem in quantum computer, to be solved in implementing quantum computer.

We can learn this from the lecture given at RIKEN and KEK in 2024 by Takafumi Tomita of Institute of Molecular Sciences [3].

"Rubidium" ( $^{87}_{37}$ Rb, Z = 37, A = 87) is used for the atom. This is an alkali atom, having 37 electrons, with (2, 8, 18, 8, 1) electrons in n = (1, 2, 3, 4, 5)-th shells, respectively, where n is the principal quantum number.

In the ground state  $|g\rangle$  of Rb, the electron in the outermost shell belongs to  $5S_{1/2}$ . This level is hyperfine-splitted (hfs) into two levels, the lower  $|0\rangle = |F1\rangle$  and the upper  $|1\rangle = |F2\rangle$ , with an energy gap  $\Delta E = 6.8[\text{GHz}] \approx 4.5[\mu\text{eV}]$ , which can constitute a single qubit  $q = (|0\rangle, |1\rangle)$ .

We know the energy levels of Hydrogen is  $E_n = -13.6/n^2 [\text{eV}]$   $(n = 1, 2, 3, \dots)$ , following Bohr's atomic model. Compared to this, the hfs is  $10^{-6}$  times smaller than the usual atomic level splitting, so it is called hyper-fine splitting.

#### 6.2 Ultra-cooling of atoms

To cool Rb atoms, we apply the laser beam with energy  $\hbar\omega_L = h\nu_L$  to them. In quantum mechanics, the energy is expressed in the words of wave, a frequency  $\nu$  or an angular frequency  $\omega = 2\pi\nu$ , as follows:

$$E = h\nu = \hbar\omega, \tag{6.1}$$

where h is the Planck constant, and  $\hbar = h/(2\pi)$  is called Dirac constant. The product of  $\hbar$  times the light velocity  $c \approx 3 \times 10^8 \text{[m/s]}$ , is approximately  $\hbar c \approx 200 \text{[eV]}[\text{nm}]$ , which is the Einstein's formula.

Assume the atom you are going to cool is a two-level atom, having a ground state  $|g\rangle$ and its excited state  $|e\rangle$  with an energy gap  $\hbar\omega_0$ . The remarkable idea here, is to apply the laser beam with a smaller energy  $\hbar\omega$  than the energy gap  $\hbar\omega_0$ , namely  $\omega_L < \omega_0$ . Then, the atom can absorb the laser photon only when they are approaching, but can not when they are receding. This is due to the *Doppler shift* of the laser energy: If the atom is moving with a velocity v, where v > 0 for approaching to or v < 0 for receding from, the laser beam. The frequency  $\omega_0$  in the rest frame of the atom differs from the frequency  $\omega_L$  in the laboratory frame,

$$\omega_0 = \omega_L \sqrt{\frac{1 + v/c}{1 - v/c}} \approx \omega_L (1 + v/c).$$
(6.2)

The atom absorbs a laser photon in the rest frame, when the absorbed energy is enough to excite the atomic level. Thus, when v is positive enough,  $(1 + v/c) = \omega_0/\omega_L > 1$ . Then, the atom slows down, by absorbing the laser photon's momentum which has the opposite direction relative to the atomic motion, that is,

$$(mv)_{\text{atom}} \to (mv)_{\text{atom}} - \hbar \omega_L/c.$$
 (6.3)

This is the Doppler cooling developed by Steven Chu's group in 1985. Even using six laser beams applied from six directions in the three dimensional space, the cooled atoms can not be at rest, but fall down by gravity. To exclude this effect by gravity, magnetic fields have to be applied, which causes the Zeeman splitting. If the energy gap of atoms moving downward is larger  $\omega_0 + \delta$ , the radiation pressure from downward laser can compensates the gravity effect. While, if the energy gap for atoms moving downwards becomes larger  $\omega_0 + \delta$ , then the larger is the radiation pressure from downward laser. Now the atoms can stay at rest. Under such scheme, the temperature lower than  $40[\mu K]$  is attained in 1987, leading to the region of Bose Einstein condensation (BEC). This method is called "Magneto-optical trap (MOT)". Doppler cooling has a lower limit,  $k_BT > k_BT_D = \hbar\Gamma/2$ , due to the deviation from the isotropy for the decay of the excited atom. The limit is determined by the decay rate  $\Gamma(|e\rangle \rightarrow |g\rangle)$ . This limit is overcome by the application of magnetic fields.

For these works on the cooling of atoms, the Nobel prize in physics (1997) was awarded [4].

## 6.3 Rough sketch of energy levels of <sup>87</sup><sub>37</sub>Rb

Rough estimation of the energy level of the electron in the n-th shell, for the atom with atomic number Z, is known by the Bohr model,

$$E_n = -13.6[\text{eV}]\frac{Z^2}{n^2}.$$
(6.4)

This gives the energy level of the ground state of  ${}^{87}_{37}$ Rb as  $E(|g\rangle)=-745$ [eV], while Rydberg states with n > 50, have energy  $E(|r\rangle) \approx 0$  (or -0.55 [eV] < E(n = 50) < 0[eV]).

The corrections from the Bohr formula, consist of (fs) fine structure coming from the relativistic corrections of  $O(10^{-3})$  [eV], the (hfs) hyper-fine structure coming from the interaction of the electron spin with the nuclear magnetic moment of  $O(10^{-4})$  [eV], and so on.

Here, the qubit is considered to be formed by two (hfs) levels of the outermost, 5S electron of Rb atom,  $(|1\rangle = |F2\rangle, |0\rangle = |F1\rangle)$ , for which the difference of energy levels is small,  $4.5[\mu \text{eV}] = 44$  [mm], having a wave length of the radio wave.

Therefore, to control the qubit  $|1\rangle \rightleftharpoons |0\rangle$  directly we have to use the laser beam with a wave length 44[mm], like UHF radio or the microwave, but we have not such low energy lasers.

Accordingly, to control the qubit, we have to prepare an intermediate higher level state  $|m\rangle$ , and control the qubit via the intermediate level. That is, to use the following processes of absorbing and emitting a laser photon as,

$$|1\rangle + \gamma \to |m\rangle \to |0\rangle + \gamma', \text{ and } |1\rangle + \gamma \leftarrow |m\rangle \leftarrow |0\rangle + \gamma'.$$
 (6.5)

Here, the intermediate state is so chosen as that photons of  $\gamma$  and  $\gamma'$  are afforded by the existent laser beams with a wave length of O(1[ $\mu$ m]).

## 6.4 Actual energy levels of ${}^{87}_{37}$ Rb and lasers to use

To implement the actual quantum computer by ultra-cold Rb atoms, we have to know the details of energy levels of Rb. We will refer to Fig.1 of the 2022 paper in [6]. The Lukin group at Harvard U. is the front runner in the implementation of the quantum computer using ultra-cold atoms.

Energy levels and lasers to be used are the followings:

1) The (hfs) gap between  $|F1\rangle$  and  $|F2\rangle$  is 6.8 [GHz]  $\approx 4.5[\mu \text{eV}]$ .

2) These two states can be raised up to and lowered from the off-resonances at 180 [GHz] below  $5P_{1/2}$ . The raising and lowering can be done by the 795 [nm] laser.

3) The upper level  $|F2\rangle$  can be raised up by the 420 [nm] laser to the off-resonance at 2 [GHz] below  $6P_{3/2}$  levels.

4) The off-resonances 2 [GHz] below  $6P_{3/2}$  can be further raised up to and lowered from the Rydberg state of  $70S_{1/2}$  with  $m_j = -1/2$ . This can be done by the 1013 [nm] laser.



Figure 6: Energy levels of Rb and radiative transitions between them

5) Trapping of cold Rb atoms to form an optical lattice is done by the 830 [nm] laser. In summary, lasers used to control qubits are

- (L1) 756 [nm] laser: exchange between ON and OFF of a qubit,  $|1\rangle \rightleftharpoons |0\rangle$ .
- (L2)  $\overline{420 \text{ [nm] and (L3) 1013 [nm] lasers: convert } |1\rangle(\text{ON}) \rightleftharpoons |r\rangle(\text{Rydberg state}).}$
- (L4) 830 [nm] laser: trap atoms, to locate the atoms on a lattice with  $O([\mu m])$  spacing.

The following rough correspondence is useful to remember,

$$\frac{1}{1,000 \text{ [nm]}} \approx 0.2 \text{ [eV]} \approx 3 \times 10^5 \text{ [GHz]} \approx \frac{1}{3 \times 10^{-3} \text{[ps]}}$$
(6.6)

In the above, the lasers are tuned not exactly on the resonance positions, but rather at offresonances. This is the *Detuning*, an important technique of optics to select a special proper motion of at as was learnt in case of the Doppler shift.

#### 6.5 Optical tweezer and optical lattice

To trap an atom at a spacially fixed point, we make a *standing wave*, by superposing waves with different phases, such as the following electric field,

$$E(x,t)_{st} = A \ e^{-i(\omega t - kx + \phi)} + A \ e^{-i(\omega t + kx - \phi)} = 2A \ e^{-i\omega t} \cos(kx - \phi),$$
(6.7)

field squared 
$$\propto |E(x,t)_{st}|^2 = 2|A|^2 \cos^2(kx - \phi)$$
. (6.8)

If an alkali atom is considered as an electric dipole with a moment d = eR, where the positive charge is composed of the nucleus plus the inside electrons, and a negative charge comes from one electron in the outermost orbit. R is the distance between the nucleus (the center of mass of the positive and negative charges) and the remaining outermost negative charge.

The interaction of electric dipole moment (edm) with the laser beam can be

$$H_{edm} = -\boldsymbol{d}(R(x)) \cdot \boldsymbol{E}(x), \tag{6.9}$$

where  $d = QR = Q(x_{+} - x_{-}).$ 

The distance R changes by the external electric field, giving a linear response,

$$\boldsymbol{d}(x) = -\epsilon(x)\boldsymbol{E}(x),\tag{6.10}$$

so that the interaction energy of the dipole reads

$$H_{edm} = -\epsilon(x)\boldsymbol{E}(\boldsymbol{x})^2 = 2\epsilon|A|^2\cos^2\left(kx - \phi\right), \qquad (6.11)$$

where  $\epsilon$  is the dielectric constant.

Now, if alkali atoms are dipoles, they are trapped at the minimum energy points, which form a optical lattice at  $kx = \phi + \pi/2(\pm 1, \pm 3, \pm 5, \cdots)$ .

It is easy to generate an optical lattice in two dimensions and three dimensions, by modulating the phase of laser beam properly in (x, y) and (x, y, z) directions. This is the mechanism of optical tweezer and the formation of optical lattices.

When the 830 [nm] laser is used as in [6],  $k = 2\pi/\lambda$ , so that adjacent Rb atoms can be aligned with a lattice spacing of 830[nm]/4  $\approx 200$ [nm].

The device to generate the optical lattice is called "AOD" (Acoustic-Optic-Defector).

#### 6.6 Spin up-down as qubit

Rather than the (hfs) splitting, it is easier to consider the qubit as a "spin" of electron, which takes up-spin state with  $s_z = 1/2$  or down-spin state with  $s_z = -1/2$ .

If we use this up-down of spin as a qubit, the magnetic dipole moment (mdm) of the electron spin interacts with the external magnetic field,

$$H_{mdm} = -g_e \ \mu_B \left(\frac{\boldsymbol{\sigma}}{2} \cdot \boldsymbol{B}(x)\right), \tag{6.12}$$

where  $\boldsymbol{\sigma}$  is the Pauli's spin matrices, with the Landé *g*-factor  $g_e$  of electron and the Bohr magneton  $\mu_B = \hbar e/m_e$ .

In this case, the qubits are controlled not by the electric field but by the magnetic field applied from outside.

There exist two possibilities, one is magnetic qubit controlled by magnetic field, the other of the atomic levels controlled by the electric field, and the mixed version of them. So far, which method is the more advantageous is not known.

Let us take a glance at the superconducting qubit. This is build by a closed circuit of superconductor with a Josephson junction. It behaves like a "LC-circuit" where the junction is a capacitor and the superconductor circuit is a non-linear inductor.[5] IBM, Google and RIKEN seem to adopt this superconducting qubit.

The Cooper pair  $(e^-(\uparrow)e^-(\downarrow))$  behaves like an electron in an artificially made atom. The non-linear inductor gives the energy levels (not equal spacing but) similar to the atom, so that we can assign the two low-lying levels as a qubit. Controling of the qubit can be done by absorbing or emitting photons like the radiative transfer of the atomic levels, or by increase or decrease of the magnetic flux passing through the superconducting circuit, since the increase or decrease of the magnetic flux introduces that of the Cooper pair's current circulating the circuit.

Now, we come back to the original possibility, the qubit by the two-level atoms, which is what Feynman considered. Feynman mentioned also the possibility of using spin as a qubit, saying the inductor is more effective than the resistance, since the former does not strongly dissipate energy, but it is difficult to use it. The difficulty which Feynman felt is now overcome by the superconducting qubit mentioned above. Recently, the implementation of the possibility of using two-level atoms, Feynman's qubits, has made a big leap, by using ultra-cold Rb atoms, so that the Feynman's two ideas (one is pessimistic and the other is optimistic to him in 1984) become now two promising ways in building quantum computers.

In comparison with (edm) Hamiltonian, we understand (mdm) is a different representation of a 3-dimensional coordinate vector, which is not the usual space coordinates  $\boldsymbol{x} = (x, y, z)$ , but is a vector represented by the two-component spinor's, two-component wave functions for spin-up and spin-down states.

Suppose the two-component spinor wave function be  $\psi = \begin{pmatrix} |\uparrow\rangle \\ |\downarrow\rangle \end{pmatrix}$ , and its hermitian conjugate be  $\psi^{\dagger} = (\langle\uparrow|, \langle\downarrow|)$ , then the vector  $\boldsymbol{x}$  can be represented by

$$\boldsymbol{x} \propto \psi^{\dagger}(x)\boldsymbol{\sigma}\psi(x).$$
 (6.13)

This correspondence will be used to define logical  $(X_L, Y_L, Z_L)$ -gates.

As a different issue, we may choose a spin as the electric dipole moment, then we have

$$H_{edm} = d_{edm} (\boldsymbol{\sigma} \cdot \boldsymbol{E}) \tag{6.14}$$

To have this Hamiltonian, CP-violation is required and is an important issue in particle physics.

#### 6.7 Basics of controlling qubits by ultra-cold atom array

In this subsection, we follow the excellent paper by Cirac and Zoller [7].

The ultra-cold atoms are assumed to be trapped by an optical lattice which is build by a standing laser beams, as was explained in the last subsection,

$$\boldsymbol{E}_{\text{trap}}(t,\boldsymbol{x}) = A \ e^{-i\omega t} (e^{i(\boldsymbol{k}\boldsymbol{x}-\phi)} + \ e^{-i(\boldsymbol{k}\boldsymbol{x}-\phi)}) = 2A \ e^{-i\omega t} \cos(\boldsymbol{k}\boldsymbol{x}-\phi).$$
(6.15)

The trapping potential  $V_{\text{trap}}(\boldsymbol{x})$  for the atom, is generated by the electric fields of laser,

$$V_{\rm trap}(\boldsymbol{x}_n) = \frac{1}{2} \times 4|A|^2 \cos^2(\boldsymbol{k}\boldsymbol{x}_n - \phi) = 2|A|^2 \left\{ (\boldsymbol{k} \cdot \boldsymbol{X}_n)^2 + \cdots \right\},$$
(6.16)

where  $X_n$  is the deviation of the CM (Center-of-Mass) coordinate of a *n*-th rapped atom, from its potential minimum  $x_n^{(0)}$ :

$$x_n = x_n^{(0)} + X_n.$$
 (6.17)

This is the harmonic oscillator potential, so we have a sound wave (phonon excitation) in each direction i = 1 - -3 as an collective excitation of atoms. Energy of the sound wave with a suffix "s" implying "sound", is

$$\hbar\omega_s = \sqrt{\frac{\text{spring const}}{\text{mass}}} = \frac{2|A||\boldsymbol{k}|_{\text{trap}}}{\sqrt{NM}}.$$
(6.18)

The paper [7] suggests to consider a collection of the CM coordinates  $\{X_n\}$  for all atoms. Then, the sound wave in atoms gives the states of the collective motion of atoms. Denote its ground state as  $|g\rangle$  and its excited states as  $|e_q\rangle$ . An additional label q = 0, 1 specifies the two ways of creating  $|e_q\rangle$  by the different polarizations of laser beams. Laser labeled by q = 0 is understood to have a Right-handed polarization  $(\gamma_R)$ , while q = 1 has a Left-handed polarization  $(\gamma_L)$ .

Here, we choose the laser energy to be smaller than the necessary energy to raise and lower the state, by  $\delta_{n,q}$ , the "detuning" discussed earlier. Furthermore, the detuning value is identified to a certain phonon excitation energy, for a specific *n*-th atom and the internal state q, such that

$$|g\rangle_n + E^{q=0}_{\text{laser}}(R) + |1\rangle_{\text{phonon}} \to |e_q\rangle_n,$$
(6.19)

$$|e_q\rangle_n \to |g\rangle_n + E_{\text{laser}}^{q=1}(L) + |1\rangle_{\text{phonon}},$$
 (6.20)

where two lasers have the same energy  $E_{\text{laser}}^{q=0,1} = E_e - E_g + \delta_{n,q}$ ,  $\delta_{n,q} = -\omega_{\text{phonon}}$ , but they have different polarizations.

The crucial point here is the <u>detuning</u>; Due to this, the extra emission and absorption of phonon is required. This is a way to control the motion of a specific bit. For example, the spontaneous emission of the excited state is prohibited unless the additional emission of phonon is allowed, which can stabilize the bit  $|1\rangle$ . Fortunately, the phonon spectrum is easily tuned by the frequency modulation of the laser used to trap atoms.<sup>2</sup>

The collective coordinate X gives an electric dipole moment d = eX, so that the electromagnetic interaction of atoms with the laser electric field  $E_{\gamma}$  can be

$$H_I = -e(\boldsymbol{X}_n(t) \cdot \boldsymbol{E}_{\gamma}(t, \boldsymbol{x}_n)), \text{ gives matrix elements}$$
(6.21)

$$H_{n,q} =_n \langle e_q | H_I | g, \text{Laser}_q, 1_{\text{phonon}} \rangle_n, \ H_{n,q}^* =_n \langle g, \text{Laser}_q, 1_{\text{phonon}} | H_I | e_q \rangle_n, \tag{6.22}$$

<sup>&</sup>lt;sup>2</sup>This detuning with the phonon excitation, is the same technique used to activate the Doppler effect; it implies that the atom moving towards the laser can be cooled down, but the atom against the laser can not. This can be understood by the detuning and the absorption of the phonon corresponding to the collective motion. The collective motion in the Doppler effect is the motion of the atom towards or against the laser beam.

where CM motion is quantized by phonon's creation and annihilation operators,

$$\boldsymbol{X}_{n}(t) = \frac{1}{\sqrt{(NM)2\omega}} \left\{ \hat{\boldsymbol{a}}_{s} e^{-i(\omega t + \phi)} + \hat{\boldsymbol{a}}_{s}^{\dagger} e^{i(\omega t + \phi)} \right\},$$
(6.23)

while the electric field of the laser photon can be expanded by the creation and annihilation operators of photons,

$$\boldsymbol{E}_{\gamma}(t,\boldsymbol{x}_{n}) = \int \frac{d^{3}\boldsymbol{K}(-i\Omega)}{\sqrt{(2\pi)^{3}2\Omega}} \sum_{q=0,1} \boldsymbol{\varepsilon}_{q}(\boldsymbol{K}) \cdot \left\{ \hat{\boldsymbol{a}}_{\gamma}^{q}(\boldsymbol{K}) e^{-i(\Omega t - \boldsymbol{K} \cdot \boldsymbol{x}_{n})} - \hat{\boldsymbol{a}}_{\gamma}^{q}(\boldsymbol{K})^{\dagger} e^{i(\Omega t - \boldsymbol{K} \cdot \boldsymbol{x}_{n})} \right\}. \quad (6.24)$$

Here, we have used small letters  $(\omega, \mathbf{k})$  for phonon and large letters  $(\Omega, \mathbf{K})$  for laser photon. The direction of the phonon's collective motion and that of the electric field of laser (along the polarization vector  $\boldsymbol{\varepsilon}$ ) has an angle  $\theta$ , giving  $(\hat{\mathbf{X}} \cdot \mathbf{K}) = K \cos \theta \equiv K_{\theta}$ .

Then, the interaction Hamiltonian of the above reactions can be written as

$$H_{n,q} = \frac{\eta}{\sqrt{N}} \frac{\Omega_{\text{Rabi}}}{2} \left( |e_q\rangle_n \langle g|ae^{-i\phi} + |g\rangle_n \langle e_q|a^{\dagger}e^{i\phi} \right) \text{ with } \eta = |K_{\theta}| / \sqrt{2M\nu_s}.$$
(6.25)

In the derivation,  $\Omega = E_{e,q} - E_g - \omega_s = E_{\text{Rabi}} - \omega_s$ , detuned from the Rabi frequency  $E_{\text{Rabi}}/\hbar = (E_{e,q} - E_g)/\hbar$ , frequency difference between the (hfs) levels, by the frequency of the CM collective motion  $\omega_s$  (phonon or sound wave). Therefore, we have to impose,  $E_{\text{Rabi}} \gg \omega_s = [\text{detuned frequency}]$ , called Rabi-Dicke-Limit (RDL).

#### 6.7.1 Hyperfine splittings and selection rule of radiative transfer

To understand why different polarization is necessary in the absorption and emission of photons, we remind of the (hfs). This splitting occurs by the interaction of total angular momentum J of electron with the nucleus spin I. The Rb atom has I = 5/2 and the 6S electron (the outermost electron of the alkali atom) has J = 1/2, which give the following (hfs) Hamiltonian, by introducing the total spin of an electron and the nucleus, F = J + I:

$$H_{hfs} = 2A_{hfs}(\boldsymbol{J} \cdot \boldsymbol{I}) = A_{hfs}\{F(F+1) - J(J+1) - I(I+1)\}$$
(6.26)

$$= A_{hfs} \left\{ F(F+1) - \frac{3}{4} - \frac{35}{4} \right\} = A_{hfs} \times \begin{cases} -3.5 \text{ for } F = 2, \\ 2.5 \text{ for } F = 3. \end{cases}$$
(6.27)

Two levels of (hfs) appar for F = 2 and 3. The energy gap between the excited state  $|e\rangle$  with F = 3 and the ground state  $|g\rangle$  with F = 2 is  $E_e - E_g = 6A_{hfs}$ .

If the nuclear spin is along the positive z-axis, then "the electron in the ground state has a down spin  $s_z = -1/2$  while in the excited state, the spin is up,  $s_z = 1/2$ ".

spin of 
$$|e\rangle = |\uparrow\rangle$$
, while spin of  $|g\rangle = |\downarrow\rangle$ . (6.28)

Now, we need the selection rules of  $\Delta J_z = 1$  and  $\Delta L = 0$ , in order for the radiative transition to occur between the two hfs states, coming from  $5S_{1/2}$ . Here, we consider  $|g\rangle = |F1\rangle$  and  $|e\rangle = |F2\rangle$  following the references [6].

This is not the electric dipole transition (E1), since (E1) transition gives  $\Delta L = 1$  and  $\Delta J = 0$ , if the circular polarization is used such as in [7]. The magnetic dipole (M1) transition

is possible, but if we stick to the dominant (E1) transition, we have to follow the selection rules  $\Delta L = 1$  and  $\Delta J = 0$ , leading to the transition between  $5S_{1/2}$  and  $5P_{3/2}$ .

Indeed the Lukin group has used this transition.

(E1) transition :  $5S_{1/2} \leftrightarrow 5P_{3/2}$  (6.29)

The circular polarization is the eigen-state of the orbital angular momentum L; if the photon moves in the z-direction, the polarization vectors point to (x, y) directions, we have

$$(\varepsilon_x - i\varepsilon_y)(X + iY) + (\varepsilon_x + i\varepsilon_y)(X - iY) = 2(\varepsilon \cdot \boldsymbol{X}).$$
(6.30)

This shows the laser with the right-polarization  $\varepsilon_R = (\varepsilon_x - i\varepsilon_y)/\sqrt{2}$  generates  $Y_{1,1}(\theta, \phi)$ , and the left-polarization  $\varepsilon_L = (\varepsilon_x + i\varepsilon_y)/\sqrt{2}$  generates  $Y_{1,-1}(\theta, \phi)$ .

If the total angular momentum J is conserved via L-S coupling in the  $5P_{3/2}$  electrons, we can understand the sophisticated Rabi oscillation used by the Lukin group. It consists of three steps,

1) the upper hfs level  $|e\rangle = |F2\rangle$  with  $s_z = 1/2$  is selectively raised by a laser  $\gamma_L$  to a detuned state of  $5P_{3/2}$ .

2) The spin of its electron is changed immediately to  $s_z = -1/2$  by L-S coupling.

3) Finally, it makes a transition to the ground state  $|g\rangle = |F1\rangle$  by emitting  $\gamma_R$ .

We have a comment on 2):

The 5P levels are split to  $5P_{1/2}$  and  $5P_{3/2}$  levels by the L-S coupling of the fine structure.

$$H_{LS} = 2A_{LS}(\boldsymbol{L} \cdot \boldsymbol{S}) = 2A_{LS}\{J(J+1) - L(L+1) - S(S+1)\}$$
(6.31)

$$= 2A_{LS} \times \begin{cases} 1 & \text{for } J = 3/2 \\ -2 & \text{for } J = 1/2. \end{cases}$$
(6.32)

The laser with right-handed or left-handed circular polarization makes the following transition:

$$|g(\uparrow)\rangle + \gamma_R = |1/2, -1/2\rangle_s \times |1, 1\rangle_R = c_1 ||3/2, 1/2\rangle_j + c_2 ||1/2, 1/2\rangle_j, \qquad (6.33)$$

$$|e_0(\downarrow)\rangle + \gamma_L = |1/2, 1/2\rangle_s \times |1, -1\rangle_L = c_3 ||3/2, 1/2\rangle_j + c_4 ||1/2, 1/2\rangle_j, \quad (6.34)$$

with C-G (Clebsh-Gordon) coefficients  $c_1 - c_4$ , so that 0 and 1 of each qubit can be mixed,

$$\langle |e_0(\uparrow)\rangle + \gamma_L ||J = 3/2, J_z = 1/2 ||g(\downarrow)\rangle + \gamma_R \rangle.$$
(6.35)

Thus, the Rabi oscillation occurs by a complex and sophisticated way.

After we know the paper [7],<sup>3</sup> we can understand how to operate the qubit made of two-level atom clearly.

# 7 Lecture 7: How to control the ultra-cold atoms by lasers

It is better to learn a little more from [7] on the operation of logic gates.

<sup>&</sup>lt;sup>3</sup>The author thanks to Jun'ichi Sone for introducing him the excellent paper [7].

#### 7.1 Operation of ultra-cold atomic QC without decoherence

Cirac and Zoller (1995) [7] gave us the very important message that there exists *qubit oper*ations without decoherence.

We start from the Hamiltonian  $H_{n,q}$  derived in the last section, in which lasers with two different polarizations  $(q = 0, 1) \equiv (R, L)$  are applied to the two level atom  $(|e_q\rangle, |g\rangle)_n$ located at site n:

$$H_{n,q} = \frac{\eta}{\sqrt{N}} \frac{\Omega_{\text{Rabi}}}{2} \left( |e_q\rangle_n \langle g|ae^{-i\phi} + |g\rangle_n \langle e_q|a^{\dagger}e^{i\phi} \right), \text{ with } \eta = |K_{\theta}| / \sqrt{2M\nu_s}, \tag{7.1}$$

where  $\nu_s$  is the frequency of phonon (sound wave) giving the collective motion of atoms in the *x*-direction. Unitary evolution  $\hat{U}_n^{k,q}$  defined by the Hamiltonian  $H_{n,q}$  for a period  $t = k\pi \frac{\sqrt{N}}{\eta \Omega_{\text{Rabi}}}$ , represents the application of the laser beam with polarization q during the period t to the *n*-th atom doing a specific collective motion:

$$\hat{U}_n^{k,q}(\phi) = e^{-ik\frac{\pi}{2}\left(|e_q\rangle_n \langle g|ae^{-i\phi} + |g\rangle_n \langle e_q|a^{\dagger}e^{i\phi}\right)},\tag{7.2}$$

where the collective motion is represented by a phonon, whose absorption and emission compensate the detuning of the laser beam energy.

The unitary transformation gives

$$\begin{pmatrix} |e_q\rangle_n|1\rangle\\|g\rangle_n|0\rangle \end{pmatrix} \to \begin{pmatrix} \cos(k\pi/2) & -ie^{i\phi}\sin(k\pi/2)\\-ie^{-i\phi}\sin(k\pi/2) & \cos(k\pi/2) \end{pmatrix} \begin{pmatrix} |e_q\rangle_n|1\rangle\\|g\rangle_n|0\rangle \end{pmatrix},$$
(7.3)

The laser beam with a polarization q = 0 controls the qubit  $(|e_0\rangle, |g\rangle)$  like  $|g\rangle \rightarrow |e_0\rangle) \rightarrow |g\rangle$ , while the laser with the other polarization q = 1 controls another qubit  $(|e_1\rangle, |g\rangle)$  like  $|g\rangle \rightarrow |e_1\rangle \rightarrow |g\rangle$ .

For a special choice of 1)  $(k = 1, \phi = 0)$  for q = 0, and 2)  $(k = 2, \phi = 0)$  for q = 1, we have, respectively,

1) operation of target bit at 
$$m$$
:  $\hat{U}_m^{1,0}(0) \begin{pmatrix} |e_0\rangle_m|1\rangle \\ |g\rangle_m|0\rangle \end{pmatrix} = -i \begin{pmatrix} 0 & 1\\ 1 & 0 \end{pmatrix} \begin{pmatrix} |e_0\rangle_m|1\rangle \\ |g\rangle_m|0\rangle \end{pmatrix}$ , and (7.4)

2) operation of control bit at 
$$n$$
:  $\hat{U}_{n}^{2,1}(0) \begin{pmatrix} |e_{0}\rangle_{n}|1\rangle \\ |g\rangle_{n}|0\rangle \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} |e_{0}\rangle_{n}|1\rangle \\ |g\rangle_{n}|0\rangle \end{pmatrix}.$  (7.5)

Here,  $\hat{U}_n^{2,1}|e_1\rangle - |e_1\rangle$  also happens, but is not used.

#### 7.1.1 CNOT gate

Now, we understand that  $\hat{U}_{mn} = \hat{U}_m^{1,0}(0)\hat{U}_n^{2,1}(0)\hat{U}_m^{1,0}(0)$  controls the 2-qubit,  $|a\rangle_n \times |b\rangle_m$ , where the bits at n and m, play the role of control bit and target bit, respectively. State vectors a, and b, take two values  $(0 \text{ or } 1) = (g \text{ or } e_0)$ , and hence we obtain

$$\hat{U}_{mn}(|a\rangle_n \times |b\rangle_m) = (\delta_{a0} - \delta_{a1})(|a\rangle_n \times |b\rangle_m).$$
(7.6)

This operation  $\hat{U}_{mn}$  can be understood as the controlled-NOT (CNOT) gate, if we express the qubit at m in a different basis,  $|\pm\rangle$  defined by

$$|\pm\rangle_m \equiv \frac{1}{\sqrt{2}} (|0\rangle_m \pm |1\rangle_m), \tag{7.7}$$

In the new basis, we have

$$\hat{U}_{mn}(|a\rangle_n \times |\pm\rangle_m) = \delta_{a0}(|a\rangle_n \times |\pm\rangle_m) + \delta_{a1}(|a\rangle_n \times |\mp\rangle_m)$$
(7.8)

showing that the *n*-th bit is a control bit and is unchanged, while the *m*-th bit is a target bit, being reversed following the CNOT operation, iff a = 1.

The change of basis can be done by acting the laser with polarization q = 0 to the *n*-th atom (control bit atom), without detuning, or without coupling to the photon, keeping the phase  $\phi$  of the standing wave, namely

$$\hat{V}_n^k(\phi) \equiv e^{-ik\frac{\pi}{2}\left(|e_0\rangle_n \langle g|e^{-i\phi} + |g\rangle_n \langle e_0|e^{i\phi}\right)}.$$
(7.9)

Notice that there is no a and  $a^{\dagger}$  in the definition.

By this operation, we can rotate the basis of qubit by angle  $k\pi/2$ ,

$$\hat{V}_{n}^{k}(\phi) \begin{pmatrix} |e_{0}\rangle_{n} \\ |g\rangle_{n} \end{pmatrix} = \begin{pmatrix} \cos(k\pi/2) & -i\sin(k\pi/2)e^{-i\phi} \\ -i\sin(k\pi/2)e^{i\phi} & \cos(k\pi/2) \end{pmatrix} \begin{pmatrix} |e_{0}\rangle_{n} \\ |g\rangle_{n} \end{pmatrix},$$
(7.10)

If we choose k = 1/2 and  $\phi = \pi/2$ , we can realize the necessary change of the basis,

$$\hat{V}_n^{1/2}(\pi/2) \begin{pmatrix} |e_0\rangle_n \\ |g\rangle_n \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} |e_0\rangle_n \\ |g\rangle_n \end{pmatrix} = \begin{pmatrix} |-\rangle_n \\ |+\rangle_n \end{pmatrix}.$$
(7.11)

Then, the operation of CNOT gate can be given by

$$\hat{C}_{mn} = \hat{V}_n^{1/2}(\pi/2)\hat{U}_{mn}\hat{V}_n^{1/2}(-\pi/2).$$
(7.12)

The more general (controlled)<sup>p</sup>-NOT gate can be given straight-forwardly. (see [7]).

#### 7.1.2 Highly entangled state

They have pointed out that a highly *entangled state* of N-atoms (qubits), can be constructed by the successive application of the quantum logic gates,

$$|\Psi\rangle = \frac{1}{\sqrt{2}} \left(|-\rangle_{N-1}|-\rangle_{N-2} \cdots |-\rangle_1|-\rangle_0 - |+\rangle_{N-1}|+\rangle_{N-2} \cdots |+\rangle_1|+\rangle_0\right)$$
(7.13)

$$= \frac{1}{\sqrt{2}} \left( |\text{alive cat}\rangle - |\text{dead cat}\rangle \right). \tag{7.14}$$

If  $N \gg 1$ , then the state becomes a macroscopic one, like a Shrödinger's "Cat", for which the quantum fluctuations are negligiblly small, so that |alive cat $\rangle$  or |dead cat $\rangle$  is determined definitely only by the measurement of a few bits of the Cat. This "Cat state" seems a key concept for the Fault-Tolerant Code (so-called "CSS" code, tolerant=braod minded) [10] in quantum computation, developed by Calderbank-Shor and Seame. Making a highly entangled state like a Shrödinger's "Cat", suppresses the decoherence and imperfectness of the quantum computation which was examined by Feynman in 1984.

Entanglement builds a strong link (correlation) between different atoms (bits). If the number of such links (*Entanglement Entropy*) is huge, then it is difficult to break all the links, leading to the suppression of the decoherence.

#### 7.2 Logical gate with Rydberg states

To implement the circuits, we have to control two and more atoms (2-qubit or more) simultaneously. However, at first sight, the dipole-dipole interaction between atoms make it impossible to control the multiple atoms simultaneously.

To overcome this difficulty, we use the Rydberg states. Even between two distant Rb atoms, the dipole-dipole interaction works. The Rydberg states  $|r\rangle$  are the states with higher principal quantum number n such as  $n \geq 50$ . They have infinitely many levels  $|r_i\rangle$   $(i = 1, 2, \dots, \infty)$  accumulated just under the ionization point, and they behave classically. Even Rydberg states  $|r_i\rangle$  and  $|r_j\rangle$  is separated with a long distance R, they contribute to the quite large dipole-dipole interactions, in addition to the Rabi oscillation energy between  $|r_j\rangle$  and the ground state  $|1\rangle$ :

$$H_{\text{Ryd}} = \frac{\hbar\Omega}{2} \sum_{i} \left( |1\rangle\langle r_i| + |r_i\rangle\langle 1| \right) - \hbar\Delta \sum_{i< j} |r_i\rangle\langle r_i|V_{ij}|r_j\rangle\langle r_j|,$$
(7.15)

with 
$$V_{ij} = \boldsymbol{d}(x_i) \frac{C}{R^6} \boldsymbol{d}(x_j = x_i + R).$$
 (7.16)

where  $\Omega = 2\pi \times 3.1$  [MHz] is the Rabi frequency between  $|1\rangle$  and  $|2\rangle$ ,  $\Delta = 2\pi \times 0.3$  [GHz] is the detuning of the laser frequency, a typical energy scale of our problem. Like the van der Waals interaction the potential is attractive, depending on  $1/R^6$ .

It is a good way to use Rydberg atoms, since the dipole-dipole interaction between them works even if they are separated at  $O[\mu m] \gg 0.1 [nm]$  (Bohr radius). However, we have to overcome a difficulty (Rydberg blockade)[13]: To excite both atoms to Rydberg states  $|g\rangle|r\rangle$  or  $|r\rangle|g\rangle \rightarrow |r\rangle|r\rangle$ , the dipole-dipole interaction shifts the excitation energy from the case of the single excitation,  $|g\rangle|g\rangle \rightarrow |g\rangle|r\rangle + |r\rangle|g\rangle$ . This difficulty has overcome, but understanding of this is, however, difficult for the author.

The description in [6] using bra and ket vectors is the same as that of creation and annihilation operators by Feynman. If we introduce the creation operator  $\hat{c}_r^{\dagger}$  of  $|r\rangle$  from  $|1\rangle$ , and its annihilation operator,  $\hat{c}_r$  (both of which are fermions), we have

$$|r\rangle = \hat{c}_r^{\dagger}|1\rangle, \ |1\rangle = \hat{c}_r|r\rangle, \ \text{and} \ |r_i\rangle\langle r_j| = \hat{c}_{ir}^{\dagger}\hat{c}_{jr}.$$
 (7.17)

Now, we can in principle, build up any logic gate, and to transport the information of the qubit at i to another qubit located at any place at j, since the dipole-dipole interaction works even between long distances. Therefore, what Feynman did by using creation and annihilation operators, is enough to form theoretically the quantum computer.

However, the actual implementation of a realistic logic circuit to work at high fidelity is a difficult issue. This was challenged by Lukin group at Harvard in U.S., the Japanese group at IMS, and others. There are a number of breakthrough in the past two years.

# 8 Lecture 8: Superconducting qubit with Josephson junction

There is another promising method to implement quantum computer, by using a *superconducting Josephson circuit*, a closed circuit of superconductor with a Josephson junction. This behaves like a "LC-circuit" in which the junction behaves as a capacitor and the superconductor circuit as a non-linear inductor.[5] [8] IBM, Google and RIKEN adopt this superconducting qubit.

The Cooper pair  $(e^-(\uparrow)e^-(\downarrow))$  carries electric charge  $(-2|e_0|)$  and behaves like an electron in an *artificial atom*. The non-linear inductor gives the energy levels similar to the atom, not equal spacing, so that we can assign the two low-lying levels as a qubit. Controlling of the qubit can be done by absorbing or emitting photons like the radiative transfer of the atomic levels, or by increase or decrease of the magnetic flux passing through the superconducting circuit, since the magnetic flux induces the Cooper pair's current circulating the circuit.

#### 8.1 Classical LC-circuit

Let us remind of the classical LC-circuit, which consists of a capacitor (condenser) with capacitance (C), and an inductor (coil) with inductance (L), without having resistance (R = 0). Provided the electric charge stored on two plates of the capacitor is  $\pm Q(t)$ , we have the electric current  $I(t) = \dot{Q}(t)$  circulating the circuit.

Therefore, the Lagrangian of the LC-circuit reads

$$\mathcal{L}_{\rm LC} = \frac{L}{2} I(t)^2 - \frac{1}{2C} Q(t)^2 = \frac{L}{2} \dot{Q}(t)^2 - \frac{1}{2C} Q(t)^2, \qquad (8.1)$$

Its equation of motion

$$L\ddot{Q}(t) + \frac{1}{C}Q(t) = L\frac{dI(t)}{dt} + \frac{Q(t)}{C} = [\text{Voltage change along the circuit}] = 0.$$
(8.2)

implies the LC circuit is the harmonic oscillator, which produces an oscillatory current I(t), and is a transmitter of the electromagnetic wave, where

$$I(t) = I_0 e^{-i\omega t}, \text{ with } \omega = 1/\sqrt{LC}.$$
(8.3)

To study the superconducting circuit (please refer to a good reference [8]), it is convenient to write the Lagrangian, in terms of the voltage  $V_x(t)$ , or the flux  $\Phi(x)$  (the time integral of the voltage  $V_x(t)$ ) at a given point (node) x in the circuit,

$$\Phi_x(t) = \int_0^t dt' \, V_x(t'). \tag{8.4}$$

This implies

$$\Phi_x(t) = \int_0^t dt' \ \int_0^x dx' \ (-1)E_{x'}(t'). \tag{8.5}$$

For a special case the circuit is closed C, then

$$\Phi_C(t) = \int_0^t dt' \oint_C dx' (-1) E_{x'}(t') = \int_0^t dt' \int d\mathbf{S} \cdot (-\mathbf{\nabla} \times \mathbf{E}) = \int_0^t dt' \int d\mathbf{S} \cdot (\partial_{t'} \mathbf{B})$$
  
= [Magnetic flux passing through C](t). (8.6)

Here, Maxwell equation (Faraday's electro-magnetic induction) has been used.

Now, we understand that  $\Phi$  introduced above implies the magnetic flux passing through the circuit C, if the circuit is closed. This corresponds to the following relation of charge as a time integral of the current,

$$Q_x(t) = \int_0^t dt' \ I_x(t').$$
(8.7)

Then, the voltage at (t, x) is

$$V_x(t) = \Phi_x(t). \tag{8.8}$$

In this way, we have another but equivalent description of the Lagrangian for the LCcircuit. Choosing the nodes 1 and 2 on the two plates of the capacitor, we have

$$\mathcal{L}_{\rm LC}' = -\mathcal{L}_{\rm LC} = \frac{C}{2} (V_1(t) - V_2(t))^2 - \frac{I_{1,2}(t)^2}{2L} = \frac{C(\dot{\Phi}_1(t) - \dot{\Phi}_2(t))^2}{2} - \frac{(\Phi_1(t) - \Phi_2(t))^2}{2L},$$
(8.9)

where we have used Q = CV.

This description also gives the harmonic oscillator.

#### 8.2 Superconducting quantum circuit

Next, we consider a superconducting circuit, made of a Josephson junction (JJ), a superconductor loop with a gap. The devise developed by U. of Tokyo in 2021 utilizes NbN (Niobium nitride) of  $T_c = 16$  [K] as a superconducting inductance, and AlN (Aluminum nitride) as a Josephson junction.

See the Figure in which Cooper Pair Box (CPB) is depicted.

The closed circuit made of the mark "X"  $(E_J)$  with the capacitance symbol "="  $(C_J)$ , describes the Josephson junction, having a gap between the superconductor loop, playing a role of capacitor for the Cooper pair  $(e^-(\uparrow) - e^-(\downarrow))$  with charge  $q = -2|e_0|$ . Here, the Cooper pair can go through the gap by the tunneling effect in quantum mechanics. In this respect, the circuit differers from the classical one, giving an anharmonic potential, and hence the superconducting circuit becomes the <u>non-linear inductor</u>.

#### 8.3 Why superconductor has no resistance

In the superconductor, the electric current flows without feeling resistance. The reason is as follows: At low temperature below a certain critical temperature  $T_c$ , Cooper pairs, pairs of two electrons  $(e^-(\uparrow)e^-(\downarrow))$  with up- and down-spins condense, and the gauge symmetry is spontaneously broken. The gauge symmetry is the symmetry to guarantee the masslessness of photon, so that the breaking of the symmetry gives photon a non-vanishing mass  $m_{\gamma} (\neq 0)$ . This is called Meissner effect.

The resistance of electric current arises when the electron looses energy by emitting photons during streaming inside the metal. If the photon becomes massive in the superconductor, however, a slowly moving electron with energy  $E_e$  less than the rest energy of the photon  $m_{\gamma}c^2$ ,  $E_e < m_{\gamma}c^2$ , can not emit photons, that is, the electron can not slow down by the resistance.

#### 8.4 Josephson relation

In deriving the Lagrangian with a non-linear potential of the superconducting quantum circuit, we use the variable  $\Phi$  (magnetic flux) suitable to describe the magnetic flux.

The kinetic term in the Lagrangian is the same as  $\frac{C(\dot{\Phi}_1(t)-\dot{\Phi}_2(t))^2}{2}$ , where  $\dot{\Phi}(t) = V(t)$ . The potential term is, however, differs from the classical case, since we have tunneling effect by Josephson.



Figure 7: Cooper Pair Box and its potential

We have denote positions 1 and 2 on the both sides of the Josephson gap.

In the following we are recommended to refer the "Feynman lecture on physics" (Quantum Mechanics). Assume the wave functions of the Cooper pair at 1 and 2 as  $\psi_1(t)$  and  $\psi_2(t)$ , which satisfies the following Schorödinger equation,

$$i\hbar \,\partial_t \psi_1(t) = eV_{12}\psi_1 + K\psi_2,,$$
(8.10)

$$i\hbar \,\partial_t \psi_2(t) = -eV_{12}\psi_2 + K\psi_1,$$
(8.11)

where  $V_{12}$  is the voltage difference between nodes 1 and 2, K represents the tunneling probability per unit time of a Cooper pair through the Josephson junction. These equations (8.10) and (8.11), can be written in terms of modulus and phase defined by  $\psi_i = n_1(t)e^{i\phi(t)}$ . Then, we have

$$(\dot{n}_1, -\dot{n}_2) = \frac{2K}{\hbar} \sqrt{n_2 n_1} \sin \phi(t),$$
(8.12)

$$\dot{\phi}_1 = -\frac{K}{\hbar} \sqrt{\frac{n_2}{n_1}} \cos \phi - \frac{eV_{12}}{\hbar}, \quad \dot{\phi}_2 = -\frac{K}{\hbar} \sqrt{\frac{n_1}{n_2}} \cos \phi + \frac{eV_{12}}{\hbar}.$$
 (8.13)

Provided that  $n_1 \approx n_2 \equiv n_J$ , the phase difference  $\phi = \phi_2 - \phi_1$  of the wave functions can be determined as

$$\dot{\phi} = \frac{2eV_{12}}{\hbar}.\tag{8.14}$$

This can be solved,

$$\phi(t) = \phi_0 + \frac{2e}{\hbar} \int_0^t dt' V_{12}(t).$$
(8.15)

The Josephson current is given by

$$I_J = 2e\dot{n}_J = I_c \sin\phi(t), \quad I_c = \frac{4eK}{\hbar}n_J, \quad (8.16)$$

where  $I_c$  is a critical current giving the maximum value of it. Eqs.(8.14) and (8.16) are called Josephson relations.

As was examined in Eq.(8.6), the variable  $\Phi$  is relevant to the magnetic flux, which can be represented as the phase difference  $\phi(t)$  of the wave functions.

This can be understood as follows: Wave function of Cooper pair satisfies the following equation apart from the tunneling interaction,

$$D_{\mu}(A)\psi(x) = (i\hbar \,\partial_{\mu} + 2eA_{\mu}(x))\,\psi(x) = 0.$$
(8.17)

When the modulus  $|\psi|$  of the wave function is constant  $\sqrt{n_i}$  =const, we have

$$\partial_{\mu}\phi(x) = \frac{2e}{\hbar}A_{\mu}(x). \tag{8.18}$$

Then, we obtain

$$\phi_x(t) - \phi_0 = \frac{2e}{\hbar} \int_0^x d\boldsymbol{x} \cdot \boldsymbol{A}(x) = \frac{2e}{\hbar} \left( \Phi_x(t) - \Phi_0(t) \right).$$
(8.19)

In this way we can replace the phase difference of the wave functions by the difference of the flux variable  $\Phi$ .

The potential energy can be estimated

$$[\text{Potential energy}] = \int_0^t V(t') I_J(t') dt' = \int_0^t dt' \,\dot{\Phi}(t) \times I_c \sin\left(\frac{2e}{\hbar}\Phi(t)\right) \tag{8.20}$$

$$= I_c \int_0^{\Phi} d\Phi \sin\left(\frac{2e}{\hbar}\Phi\right) = \frac{\hbar I_c}{2e} \left(1 - \cos\frac{2e}{\hbar}\Phi\right).$$
(8.21)

Now, we have arrived at the Lagrangian for the Cooper pair box (CPB) depicted in Figure, as follows:

$$\mathcal{L}_{\rm CPB} = \frac{C_g (\dot{\Phi} - V_g)^2}{2} + \frac{C_J \dot{\Phi}^2}{2} - E_J \left( 1 - \cos \frac{2e\Phi}{\hbar} \right), \tag{8.22}$$

where the Josephson energy is given by

$$E_J = \frac{\hbar I_c}{2e}.\tag{8.23}$$

This CPB gives an artificial atom, having the anharmonic potential

$$V(\Phi) = E_J \left[ 1 - \cos\left(\frac{2e}{\hbar}\Phi\right) \right]$$
(8.24)

$$=E_{J}\left[\frac{1}{2}\left(\frac{2e}{\hbar}\Phi\right)^{2}-\frac{1}{4!}\left(\frac{2e}{\hbar}\Phi\right)^{4}+\frac{1}{6!}\left(\frac{2e}{\hbar}\Phi\right)^{6}-\cdots\right].$$
(8.25)

It is important to know the potential of CPB or artificial atom, is periodic. Thus, there are infinite number of minima at  $\Phi = (h/2e)N$  (N=number of quantized vortices through the circuit), and hence, the soliton solutions appear which connect different minima. Let us remind of the Mandelstam's duality between the sine-Gordon model and the massive Thirring model.

Then, It seems interesting to study the quantized CPB or the artificial atom, in terms of the fermionic "massive Thirring model". The periodic potential also suggests the appearance of the band structure in the artificial atom array.

### 9 Quantum error correction (QEC)

The qubit is described by a quantum mechanical wave function  $|\psi\rangle$  which is easily modified by the perturbation from outside circumstances. The perturbation is given by a unitary transformation  $U(\alpha)$  with complex parameters  $\alpha$ . This is the origin of quantum errors for the quantum computer:

$$[\text{Quantum Errors (QE)}] : |\psi\rangle \to |\psi'\rangle = U(\alpha)|\psi\rangle.$$
(9.1)

How to detect these errors and correct them, is the important issue in the quantum computation.

#### 9.1 Fault-tolerant quantum computing

If we could know the wave function  $|\psi\rangle$  for a system of k atoms in a Hilbert space  $\mathcal{H}$ , then we could eliminate the errors (or perturbations) in the wave function of the k-qubits. Unfortunately, we can't do that.

Let us examine whether the extension of the Hilbert space  $\mathcal{H}$  can solve the difficulty. More explicitly, we embed  $\mathcal{H}$  into a larger Hilbert space  $\mathcal{H}'$  of n atoms (n-qubit, n > k), and seek the possibility for which the embedded state (called Encoded state or "logical words")  $|\psi_L\rangle = En|\psi\rangle$  is known definitely. In some cases this works, and the errors can be eliminated in the larger Hilbert space. This is the "Fault-Tolerant quantum computing".

The encoded state  $|\psi_L\rangle$  before destroyed by the errors, is a vector in  $\mathcal{H}'$  without having the informations of the extra (n-k) atoms. This means we can find (n-k) independent projection operators,  $(P_1, P_2, \cdots, P_{n-k})$ , so that the state vector may be invariant under them:

$$|\psi_L\rangle = P_1 P_2 \cdots P_{n-k} |\psi_L\rangle. \tag{9.2}$$

We can assume that the constraints imposed by the projections be commutative, then we can express

$$P_i = \frac{1+M_i}{2}$$
, with  $[M_i, M_j] = 0$ ,  $(M_i)^2 = 1$ , (9.3)

where all Ps or Ms are chosen to be linearly independent.

These Ms are called "Stabilizers", which form a group,  $S = \{M_1, M_2, \cdots, M_{n-k}\}$ .

The original state  $|\psi\rangle$  has eigen-value 1 for all the stabilizer elements  $\{M_i\}_{i=1-(n-k)}$ . Therefore, it can be a syndrome of errors if the state has negative eigen-values for some Ms. To correct all the quantum errors, any perturbation caused by 3n generators of the unitary transformation,  $G_{\alpha}$  ( $\alpha = 1 - 3n$ ) =  $\{(\sigma^i)_a | i = 1 - 3, a = 1 - n\}$ , should be detected by the negative eigen-values for Ms. Including the identity operator  $I^n$ , without error in the *n*-qubits, the total number of operators to be detected is 3n + 1, which can be classified by the signs (positive and negative) of (n - k) eigen-values of the stabilizer generators,  $M_i = \pm 1$  [i = 1 - (n - k)]. For this to occur, we need at least the following condition,

$$3n+1 \le 2^{n-k} \Leftrightarrow n - \ln_2(3n+1) \ge k. \tag{9.4}$$

It is, of course, a difficult task to find the (QEC) code explicitly. If we find the code, we can do the following.

The error correction is possible means that for any perturbation  $U(\alpha)$  in the original Hilbert space  $\mathcal{H}$  can be corrected by a suitable choices of encoding En and decoding  $De = (En)^{-1}$  in the extended Hilbert space  $\mathcal{H}'$ . Namely,

$$|\psi_L\rangle = En U(\alpha)En^{-1}|\psi_L\rangle = \left(En U(\alpha)En^{-1}\right)|\psi_L\rangle.$$
(9.5)

To reproduce the condition (9.2) of invariant under projections, we have

$$En U(\alpha)En^{-1} = \prod_{i} P_i, \qquad (9.6)$$

Then, we can detect errors and correct them by applying the inverse unitary transformation as follows:

[Quantum Error Correction (QEC)]: 
$$|\psi'\rangle \to |\psi\rangle = U(\alpha)^{-1}En^{-1}|\psi'_L\rangle.$$
 (9.7)

Our superficial discussion in the above is far from the real existence theorem of ECC. To know it, please read seriously [9] and [10].

What we can do here is to give and understand the two typical (QEC) codes, one is the correction of error in 1-qubit code [[5, 1]], by extending 1-qubit to 5-qubit [11], and the other [[8, 3, 2]] is the three dimensional "color code", used in the implementation of the quantum computer by the Lukin group [12].

#### 9.2 X, Y, Z gates

The unitary transformation  $\hat{U}$  of a single qubit  $|q\rangle = \begin{pmatrix} |1\rangle \\ |0\rangle \end{pmatrix}$ , is generated by three Pauli matrices  $(\sigma^1, \sigma^2, \sigma^3) \equiv (X, Y, Z)$  as follows:

$$|q'\rangle = \hat{U}|q\rangle, \ \hat{U} = e^{-i(\alpha X + \beta Y + \gamma Z)}$$
 with real parameters  $(\alpha, \beta, \gamma),$  (9.8)

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$
(9.9)

These three 2x2 matrices are called Pauli matrices, which satisfy the following relations,

$$X^{2} = Y^{2} = Z^{2} = 1, \ XY = iZ, \ YZ = iX, \ ZX = iY.$$
(9.10)

The operations of (X, Y, Z) on a qubit are called (X, Y, Z) gates or Pauli gates. The identity operation is denoted by I.

The logic gate (X, Y, Z) is applied to each qubit, or to each (real or artificial) atom. For example, a 5-qubit state made of 5 atoms  $(a_1, a_2, \dots, a_5)$ , with a wave function  $\psi \rangle = |a_1\rangle|a_2\rangle\cdots|a_5\rangle$ , the logical operation is such as

$$\hat{O} = I_{a_1} X_{a_2} Y_{a_3} I_{a_4} Z_{a_5}. \tag{9.11}$$

Therefore, a n-bit state is perturbed from outside quantum mechanically, as

$$|\psi\rangle \to |\psi'\rangle = \left(I - i\sum_{a=1}^{n} (\alpha_a X_a + \beta_a Y_a + \gamma_a Z_a) + \dots |\psi\rangle\right)$$
(9.12)

$$= \left(I + \sum_{(a;b;c)} \alpha_{a;b;c} (X_{a_1} \cdots X_{a_p}) (Y_{b_1} \cdots Y_{b_q}) (Z_{c_1} \cdots Z_{c_r})\right) |\psi\rangle, \tag{9.13}$$

where  $(a; b; c) = (a_1, \dots, a_p; b_1, \dots, b_q; c_1, \dots, c_r)$  denotes a subset of n atoms (qubits).

#### 9.2.1 Unitary rotation by finite angle $\theta$

Let us consider the time development of a qubit in quantum mechanics, with a Hamiltonian  $H_{\rm rot}$  which rotates the qubit  $|q\rangle = (|1\rangle, |0\rangle)^T$  by an angle  $\theta$ :

$$R(\theta) = e^{-iH_{\rm rot}\theta}, \text{ with } \theta = \Omega t.$$
 (9.14)

Here the rotation angle is equal to the phase shift  $\theta = \Omega t$  for the laser with angular frequency  $\Omega$  to obtain after illuminating the atom for t [s]. Corresponding to the Hamiltonian defined by (X, Y, Z) gates, we have the operation of the finite rotation, which is denoted by  $(X(\theta), Y(\theta), Z(\theta))$  in the references of quantum computers.

$$X(\theta) = R_x(\theta) = e^{-iX\theta} = 1 - iX\theta + \frac{1}{2!}(-iX\theta)^2 + \frac{1}{3!}(-iX\theta)^3 + \dots = \cos\theta - iX\sin\theta,$$
(9.15)

where  $X^2 = 1$  is used. Pauli gates satisfy  $Y^2 = Z^2 = 1$ , we have similarly,

$$Y(\theta) = R_y(\theta) = \cos \theta - iY \sin \theta, \ Z(\theta) = R_z(\theta) = \cos \theta - iZ \sin \theta.$$
(9.16)

Following Feynman, we can use the creation and annihilation operators  $(\hat{b}, \hat{b}^{\dagger})$ , and write

$$X = \hat{b} + \hat{b}^{\dagger}, \ Y = i(\hat{b} - \hat{b}^{\dagger}), \ Z = \hat{b}^{\dagger}\hat{b} - \hat{b}\hat{b}^{\dagger}.$$
(9.17)

#### 9.2.2 Hadamard gate H

Sometimes the symbol H appears in the diagram of logical gates for qubits. Don't misunderstand it as Hamiltonian, but this is "Hadamard" gate H converting the qubit bases, from  $(|1\rangle, |0\rangle)^T$  to  $(|+\rangle, |-\rangle)^T$ .

$$H: \begin{pmatrix} |+\rangle \\ |-\rangle \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \begin{pmatrix} |1\rangle \\ |0\rangle \end{pmatrix}.$$
(9.18)

For example, H appears like  $H \cdot \text{CNOT}_{a,b} \cdot H = \text{CNOT}_{b,a}$ , where the first qubit a in  $M_{a,b}$  is controller and the second bit b is a target, following Feynman. This is equivalent to the basis changing operator of  $\hat{V}^{1/2}(\pi/2)$  in [7]

Now, we can understand any logical qubits shown in various references in quantum computers.

#### 9.2.3 Transversal gate T

Sometimes the following "transversal gate" T appears, which is a unitary operator, but not a Pauli gate, and det  $T \neq 1$ ,

$$T = \begin{pmatrix} 1 & 0\\ 0 & e^{i\pi/4} \end{pmatrix}. \tag{9.19}$$

#### 9.3 [[5, 1]] code

The simplest example of Fault-tolerant code, is QEC for a single qubit  $\psi \rangle = |a\rangle = |1\rangle$  or  $|0\rangle$ . We refer to [11].

This is originally a single qubit (k = 1). To correct the error, we have to extend a single qubit to 5-qubits  $(n = 5, \text{ and we obtain the logical code } |\psi_L\rangle = |a_1\rangle|a_2\rangle \cdots |a_5\rangle$ .

We have to discriminate whether there are errors or not. No error means the perturbation is *I*. Errors are generated by rotations  $(X_a, Y_a, Z_a)$  at a = 1 - 5, and we have to know the place *a* of the error occurred, and the type of them, *X* or *Y* or *Z*. This can be measured by the sign of eigen-values for properly defined stabilizers  $S = \{M_1, M_2, \dots\}$ .

The proper choice is the following four stabilizer generators  $\{M_1, M_2, M_3, M_4\}$ , given by

$$M_1 = XZZXI, \ M_2 = IXZZX, \ M_3 = XIXZZ, \ M_4 = ZXIXZ.$$
(9.20)

We prepare "X and Z operations" for the logical qubit as  $X_L$  and  $Z_l$ ,

$$X_L = XXXXX, \ Z_L = ZZZZZ. \tag{9.21}$$

Then, the original qubit is encoded as a logical 5-qubit,

$$|0_L\rangle = \prod_{i=1}^4 \frac{1+M_i}{2}|00000\rangle, \ |1_L\rangle = X_L|0_L\rangle.$$
 (9.22)

Here, the following relations hold

$$[M_i, X_L] = M_i, Z_L] = 0, \{X_L, Z_L\} = 0, \text{ and}$$
 (9.23)

$$Z_L|0_L\rangle = |0_L\rangle, \ Z_L|1_L\rangle = -|1_L\rangle.$$
(9.24)

(Note: In the definition of a qubit here, the role of  $|0\rangle$  and  $|1\rangle$  are exchanged from our definition used so far.)

Making a list of eigenvalues of the measurements  $\{M_1 - M_4\}$  about the 16  $(1+3\times 5 = 16)$  operators generating no error and errors, we understand that all the errors can be detected and corrected. It is consistent, since the number of variables and equations are equal; the former is the total number  $2^4 = 16$  of sign differences for four eigen-values, and the latter is  $16 = 1 + 3 \times 5$ , discussed in the above.

## 9.4 [[8, 3, 2]] code

Next, we go to [[8, 3, 2]] code, by referring [12]. This code is defined geometrically on a cube. See Figure 8 in which the eight vertices are numbered.



Figure 8: [[8, 3, 2]] color code. In referring papers by Lukin group, the assigned number of vertices should be increased by 1, namely (12345678) from (01234567) in the figure.

The original 3-qubit is placed on the three surfaces or three edges, while the 8-qubit extended for QEC, is placed on the eight vertices of a cube.

So, two numbers 8 and 3 in the code name can be understood, but what is the last number 2?

Following [12], 3-qubit description is called "logical", while 8-qubit one is "physical". Operators acting on the former logical qubits (3-qubits) are denoted with "overline", while the operators without overline are the action on the physical qubits (8-qubits).

The physical qubits (given by eight atoms) reside on the eight <u>vertices</u>, with the labeling in the Figure 8. The operators for the three logical qubits are located on three <u>surfaces</u> (0123), (0143) and (0246) around the vertex 0, or three <u>edges</u> (04), (02), and (01). The three surfaces and three edges are orthogonal (or dual), respectively.

The generators of the stabilizer are given on the surfaces by

$$\mathcal{S} = \left\{ \prod_{i=1}^{8} X_i, \ Z_0 Z_1 Z_2 Z_3, \ Z_4 Z_5 Z_6 Z_7, Z_0 Z_1 Z_4 Z_5, Z_0 Z_2 Z_4 Z_6 \right\}.$$
(9.25)

The operators on the logical 3-qubits are given by

$$\overline{X}_1 = X_0 X_1 X_2 X_3, \ \overline{X}_2 = X_0 X_1 X_4 X_5, \ \overline{X}_3 = X_0 X_2 X_4 X_6, \tag{9.26}$$

$$\overline{Z}_1 = Z_0 Z_4, \ \overline{Z}_2 = Z_0 Z_2, \ \overline{Z}_3 = Z_0 Z_1.$$
 (9.27)

In addition to the (X, Y, Z) gates we consider the following transversal gate T defined by

$$T = \begin{pmatrix} 1 & 0\\ 0 & e^{i\pi/4} \end{pmatrix} \tag{9.28}$$

with which the logical  $\overline{\text{CCZ}}$  gate can be give by

$$\overline{\text{CCZ}} = T_0 T_1^{\dagger} T_2^{\dagger} T_3 T_4^{\dagger} T_5 T_6 T_7^{\dagger}.$$
(9.29)

Let us check the necessary condition of (QEC) in (9.4). Here k = 3 and n = 8, this condition holds

$$3n + 1 = 25 < 2^{n-k} = 2^5 = 32. (9.30)$$

Of course, the explicit verification of how QEC is fulfilled, should be examined. This was of course done.

Now, we can in principle, build up any logic gate, and transport the information of the qubit at i to j, since the dipole-dipole interaction works even between long distances. Therefore, what Feynman did is enough to understand theoretically the quantum computer.

However, the implementation for an actual logical circuit to work at high fidelity, is a difficult task. This was challenged by Lukin group at Harvard in U.S., the Japanese group at IMS, and others. There appeared a number of breakthrough in the past two years.

## 10 Epilogue

We are very happy, even if we have just cleared the elementary stage of quantum computer, and finally stand at the entrance of this active and interesting region. We have learnt from Feynman that there exist a number of difficulties before implementing the real machine. Probably the quantum machine shows it strength, when the characteristic features of quantum mechanics work effectively. They are 1) *interference* of different waves which is familiar from the path integration, and 2) *entanglement* which seems to protect the machine from the decoherence.

Honestly speaking, the author has a clear intuition on the former, but not on the latter. In terms of the interference, we can understand why the quantum computer is extremely rapid and effective, in considering the measurement of the crystal type. It is known, immediately after we focus a proper light on the crystal and observe the interference pattern of Bragg.

"Is there a similar intuitive understanding of the entanglement?"

To make an entanglement, we have to build a linkage between the states of two different particles (atoms or spins), such as to keep the total spin of them to zero. To obtain a highly entangled state, we have to construct the extremely large number of linkages. How can we do it? To make a linkage one by one or to detect it one by one, is not so difficult. This is like a cat is born and grows following the encoded program in DNA. But, it seems not so easy to construct and detect the *entanglement at the macroscopic scale*.

In this situation, can a certain *randomness* be a candidate mechanism to protect the decoherence? Let us remind of the spin-glass; it is quite similar to QEC. For example, the SYK model is a kind of spin glass having random interactions [16]. The randomness introduces a *replica symmetry* [15], which extends the Hilbert space to a infinite number of its replicas, as is similar to the extension of the logical bits to the physical bits. The spin-glass becomes stable not in the usual sense, but in a configuration of extended (replica) spins, breaking the replica symmetry.

As for the structure formation, the cosmology is easier than the biology of creating the cat. In the early universe, the quantum fluctuation occurs which gives a seed of attracting particles and forming galaxies. That is, the fluctuation is self-organized to form the order [14]. We know from the cosmology that the attractive nature of gravity is crucial in the galaxy formation. It is amazing that the spin glass model of SYK supports the emergence of gravity.

Even from this elementary discussion, we recognize that important concepts, such as entanglement, decoherence, structure formation, spin-glass, QEC and others are mutually related. Therefore, the quantum computation is expected to contribute to the other issues in physic, as well as to be influenced from them.

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