Full quantum treatment of Rabi oscillation driven by pulse train and its application in ion-trap quantum computation

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Abstract. Rabi oscillations of two-level system driven by pulse train is a basic process involved in quantum computation. We give a full quantum treatment of this process, and show that the population inversion of this process collapses exponentially, has no revival phenomenon, and has a dual-pulse structure in every period. As an application, we investigate the significance of above results in ion-trap quantum computation. We find that when the wavelength of the driving field is of the order $10^{-6}$ m, the lower bound of failure probability is no less than $10^{-2}$ after $10^2$ operations. It means that in Cirac-Zoller scheme, after about $10^2$ CNOT gates, the failure probability arrives at $10^{-2}$. This value is about the generally-accepted threshold in one error-correction period in fault-tolerant quantum computation.
1. Introduction

The presented quantum algorithms show that quantum computer (QC) can solve several famous problems intractable on classical computers [1], then challenge most public-key cryptosystems in use [2, 3]. Many proposals for implementing QC have been put forward. Among them, the cold ion trap scheme (Cirac-Zoller scheme) [4] is the earliest and most promising one, e.g., a scalable, multiplexed ion trap for quantum information processing has been demonstrated [5]. Implementation of quantum logic gates in this scheme is realized via Rabi oscillation of ions driven by pulse train of laser fields. The interaction of a single atom with radiation field is a basic interaction in physics. In [6], a nonperturbative fully quantum-theoretical analysis describing the transient spontaneous emission of an initially excited two-level atom in a one-dimensional cavity with output coupling is presented. In [7], they present observations of quantum dynamics of an isolated neutral atom stored in a magneto-optical trap.

The theoretic measure adapted in [4] is a typical one which takes the laser field as a classical field. However, considering the quantum nature of the driving field, one may get results which is different from the result under classical treatment. There are generally two ways to take account of the quantum nature of the field. One is to add quantum fluctuations to the classical treatment [8]. However, there are many operations in quantum computation, then in this case whether this method is suitable is still to be considered. The other way is to quantize the field and work out the result [9]. To do this, we first consider the Rabi oscillation driven by quantized pulse train. This is a basic atom-photon interaction process, and quantum computation is only one application of it. Then we can analyze the failure probability in ion-trap QC, and have further discussions.

Rabi oscillation driven by a quantized continuous-wave (cw) field, accompanied by collapse-revival phenomenon [10, 11, 12, 13], is a typical phenomenon of atom-photon systems. However, Rabi oscillation driven by quantized pulse train has not been fully investigated. Conceivably, it may have different phenomena compared with that driven by a cw field.

Fault-tolerant quantum computation (FTQC) allows the computer to work normally even when its elementary components are imperfect. However, the threshold theorem in FTQC requires the failure probability of each components below some threshold [14]. Then we can compare the failure probability with the value of threshold, and reach some meaningful conclusion in quantum computation [9].

This paper is arranged as follows: in Section 2 we describe a method to deal with quantum transformation of a two-level system after one coherent pulse, which expresses the relationship between the density matrices for the two-level system before and after one coherent pulse. In Section 3 we investigate the properties of Rabi oscillation driven by pulse train. In Section 4 we study this kind of Rabi oscillation in ion-trap quantum computation, and get the failure probability. In Section 5 we give out some discussions. In Section 6 some conclusions are reached.
2. Quantum transformation of a two-level system involving one coherent pulse

2.1. Modeling

The two-level system driven by repeated pulses is an open system, the usual way to deal with such a system is Kraus summation and master equation method. However, for the specific problem here, which cannot be easily solved with those methods, we study it in this way: after a single pulse, we get the density matrix for the whole system (including a two-level system and the laser field), then obtain the reduced density matrix for the two-level system. We can get the relation for the state of the two-level system before and after the pulse, then the state of the two-level system after repeated pulses can be get.

In [8, 15], they use the Jaynes-Cummings model (JCM) [16] for the case where an atom in the free space interacts with laser field. However, the JCM is the model to describe the interaction of atom and single-mode field in a cavity. Actually, there are some discussions [17, 18, 19] on the validation of the JCM in the multi-mode case. For example, in the paper by Enk and Kimble [15], at section 2.3 “Atom-light interaction”, they considered the case where an atom in free space interacts with a laser field, making use of Hamiltonian of JCM in Eq.(10). They also pointed out that the Hamiltonian in Eq. (10) in the paper is valid for atoms in free space for less than one Rabi period, but there is no strict proof.

We analyze the issue as follows: the sources of decoherence can generally lead to certain amount of failure probability on a single qubit or a pair of qubits. After many operations on the same qubit (or the same pair of qubits), the failure probability will generally accumulate to reach the threshold in the threshold theorem of FTQC. The corresponding operation number is the upper bound of operation number in one error-correction period when the given source of decoherence exists. Each source of decoherence considered can generally give corresponding upper bound of operation number, but this upper bound can be enlarged by technique improvement. When the upper bound increased to a huge value, it is actually not a bound.

The decoherence caused by field quantization can also give its upper bound of operation number. It is obtained theoretically, thus cannot be enlarged by technique improvement. The calculation of this decoherence should include the interaction of all modes in the radiation field with the two-level system. When using JCM, only one mode of the field is considered, and can also give an upper bound of operation number $\beta_1$. The accurate upper bound of operation number from field quantization $\beta < \beta_1$, because the spontaneous emission induced by vacuum modes is not considered in JCM. Then if we use JCM to estimate the upper bound of operation number in one error-correction period from field quantization, we can get meaningful results. The two-level system driven by pulse train can be described as

$$H = \hbar g \left( e^{i\phi} \sigma_+ a + e^{-i\phi} a^\dagger \sigma_- \right),$$

(1)
where $g$ is the coupling constant, $\phi$ is the beam phase, $\sigma_+$ and $\sigma_-$ are the raising and lowering operators of the two-level system, and $a^\dagger$ and $a$ the creation and annihilation operators of photons, respectively. Then the unitary time-evolution operation is given by

$$U(t) = \cos (gt\sqrt{a^\dagger a + 1}) |1\rangle\langle 1| + \cos (gt\sqrt{a^\dagger a}) |0\rangle\langle 0|$$

$$-i \left[ e^{i\phi} \frac{\sin (gt\sqrt{a^\dagger a + 1})}{\sqrt{a^\dagger a + 1}} a |1\rangle\langle 0| + e^{-i\phi} a^\dagger \frac{\sin (gt\sqrt{a^\dagger a + 1})}{\sqrt{a^\dagger a + 1}} |0\rangle\langle 1| \right],$$

(2)

with $|0\rangle$ and $|1\rangle$ the ground and excited state of the two-level system respectively.

Generally, the initial state of the whole system is $|\psi(0)\rangle = \sum_{n=0}^{\infty} c_n |n\rangle \otimes (\alpha|0\rangle + \beta|1\rangle)$, where $|c_n|^2 = \frac{e^{-\frac{n\pi}{\hbar^2}}}{n!}$, and $|\alpha|^2 + |\beta|^2 = 1$. A single qubit gate is usually implemented through a $k\pi$ pulse in Cirac-Zoller scheme, whose duration $t_0$ satisfies $gt_0\sqrt{n} = \frac{k\pi}{2}$ [15], with $n$ the mean number of photons in the pulse. After a $k\pi$ pulse, the state for the two-level system and laser field is

$$|\psi_1\rangle = \alpha \left\{ \sum_{n=0}^{\infty} c_n \left[ \cos\left(\frac{k\pi\sqrt{n}}{2\sqrt{n}}\right)|0, n\rangle - i\frac{\sqrt{n}}{n} \sin\left(\frac{k\pi\sqrt{n}}{2\sqrt{n}}\right)|1, n-1\rangle \right] \right\}$$

$$+ \beta \left\{ \sum_{n=0}^{\infty} c_n \left[ \cos\left(\frac{k\pi\sqrt{n+1}}{2\sqrt{n}}\right)|1, n\rangle - i\frac{\sqrt{n}}{n} \sin\left(\frac{k\pi\sqrt{n+1}}{2\sqrt{n}}\right)|0, n+1\rangle \right] \right\}.$$ (3)

The corresponding density matrix for the state in (3) is $\rho_\text{total}^{(1)} = |\psi_1\rangle\langle \psi_1 |$. This matrix contains the information of both the two-level system and the field, but we are interested only in the two-level system. Thus we obtain the reduced density matrix

$$\rho^{(1)} = \left[ |\alpha|^2 S_4 + \frac{1}{2} (|\alpha|^2 - |\beta|^2) e^{i\phi} S_2 + |\beta|^2 (1 - S_6) \atop \alpha^* \beta^* S_5 + i (|\alpha|^2 e^{i\phi} S_1 - |\beta|^2 e^{-i\phi} S_7) + \alpha^* \beta S_3 \atop \alpha^* \beta S_5 - i (|\alpha|^2 e^{i\phi} S_1 - |\beta|^2 e^{-i\phi} S_7) + \alpha^* \beta S_3 \atop |\alpha|^2 (1 - S_4) - \frac{1}{2} (|\alpha|^2 - |\beta|^2) e^{i\phi} S_2 + |\beta|^2 S_6 \right],$$

where

$$S_1 = \sum_{n=0}^{\infty} \frac{e^{-\frac{n\pi}{\hbar^2}} n!}{n!} \sqrt{\frac{n}{n+1}} \sin\left(\frac{k\pi\sqrt{n+1}}{2\sqrt{n}}\right),$$

$$S_2 = \sum_{n=0}^{\infty} \frac{e^{-\frac{n\pi}{\hbar^2}} n!}{n!} \sqrt{\frac{n}{2(n+1)}} \sin\left(\frac{k\pi\sqrt{n+1}}{2\sqrt{n}}\right),$$

$$S_3 = \sum_{n=0}^{\infty} \frac{e^{-\frac{n\pi}{\hbar^2}} n!}{n!} \sqrt{\frac{n}{n+1}} \sin\left(\frac{k\pi\sqrt{n+1}}{2\sqrt{n}}\right),$$

$$S_4 = \sum_{n=0}^{\infty} \frac{e^{-\frac{n\pi}{\hbar^2}} n!}{n!} \cos^2\left(\frac{k\pi\sqrt{n}}{2\sqrt{n}}\right),$$

$$S_5 = \sum_{n=0}^{\infty} \frac{e^{-\frac{n\pi}{\hbar^2}} n!}{n!} \cos\left(\frac{k\pi\sqrt{n}}{2\sqrt{n}}\right) \cos\left(\frac{k\pi\sqrt{n+1}}{2\sqrt{n}}\right),$$

$$S_6 = \sum_{n=0}^{\infty} \frac{e^{-\frac{n\pi}{\hbar^2}} n!}{n!} \cos^2\left(\frac{k\pi\sqrt{n+1}}{2\sqrt{n}}\right),$$

(4)
\[ S_T = \sum_{n=0}^{\infty} \frac{e^{-\bar{n}n}}{n!} \sqrt{\frac{n}{\bar{n}}} \cos\left(\frac{k\pi n + 1}{2\sqrt{n}}\right) \sin\left(\frac{k\pi \sqrt{n}}{2\sqrt{n}}\right). \]

2.2. Transforms of the density matrix after a coherent pulse

Consider the relationship between \( \rho^{(1)} \) and the density matrix of corresponding initial state \( \rho^{(0)} = |\psi(0)\rangle \langle \psi(0)| \). For a two-level system, the density matrix \( \rho \) satisfies the condition \( \rho = \frac{1}{2}(I + r \cdot \sigma) \) [14], \( r \) is the Bloch vector for state \( \rho \), \( |r| \leq 1 \), \( \sigma = \left[ \begin{array}{ccc} \sigma_x & \sigma_y & \sigma_z \end{array} \right]^T \).

Let \( r^{(m)} = \left[ r_x^{(m)} \ r_y^{(m)} \ r_z^{(m)} \right]^T \) denotes the Bloch vector of \( \rho^{(m)} \). An arbitrary trace-preserving quantum operation is equivalent to a map of the form \( r \xrightarrow{\xi} r' = Mr + c \) [14], here \( M \) and \( c \) contain the properties of the system and are independent of the state. Based on this, it can be seen that \( r^{(1)} = Mr^{(0)} + c \), here \( c = \left[ \begin{array}{ccc} 0 & S_7e^{-i\phi} - S_1e^{i\phi} & S_4 + S_6 - 1 \end{array} \right]^T \),

\[ M = \left[ \begin{array}{ccc} S_3 + S_5 & 0 & 0 \\ 0 & M_1 & 0 \\ 0 & 0 & M_2 \end{array} \right], \]
\[ M_1 = \left[ \begin{array}{ccc} S_5 - S_3 & -(e^{i\phi}S_1 + e^{-i\phi}S_7) & 0 \\ e^{i\phi}S_1 + e^{-i\phi}S_7 & S_4 - S_6 & 0 \\ 0 & 0 & 0 \end{array} \right]. \]

then \( r^{(m)} = Mr^{(m-1)} + c \).

2.3. Calculation of the sums in the density matrix

It is necessary to get accurate values of \( S_i \ (i = 1, \cdots, 7) \) to evaluate the behavior of pulse train. The usual algorithm (saddle-point approximation) can only reach a precision of \( 1/\sqrt{n} \). Our algorithm achieving any given precision instead of the usual algorithm is as follows.

Suppose \( \bar{n} \) is not small, for the sum
\[ \sum_{n=0}^{\infty} \frac{e^{-\bar{n}n}}{n!}f_{i0}(n, \bar{n}, k), \]

(1) Substitute \( n \) in \( f_{i0}(n, \bar{n}, k) \) with \( (x+1)\bar{n} \), we get \( f_{i1}(x, \bar{n}, k) = f_{i0}\left((x+1)\bar{n}, \bar{n}, k\right) \).

(2) Do Taylor expansion to \( x^p \) for \( f_{i1}(x, \bar{n}, k) \) at \( x = 0 \), and get \( f_{i2}(x, \bar{n}, k) \).

(3) Since sum \( \sum_{n=0}^{\infty} \frac{e^{-n\bar{n}}n^k}{n!} \) can be get accurately, we replace \( x \) in \( f_{i2}(x, \bar{n}, k) \) by \( \frac{n-x}{\bar{n}} \) and get \( f_{i3}(n, \bar{n}, k) \).

(4) Use \( f_{i3}(n, \bar{n}, k) \) instead of \( f_{i0}(n, \bar{n}, k) \) in the expression of \( S_i(\bar{n}, k) \) to calculate the new sum and get \( f_{i4}(\bar{n}, k) \).

(5) Substituting \( \bar{n} \) into \( f_{i4}(\bar{n}, k) \), we obtain a high-precision result of the original sum \( S_i(\bar{n}, k) \). The value for \( S_i \ (i = 1, \cdots, 7) \) in the cases where we expand \( f_{i1}(x, \bar{n}, k) \) to \( x^{10} \) and \( x^{15} \) are compared in Table 1.

The precision of the sums \( S_i(i = 1, 2, \cdots, 7) \) is ensured by the following theorem:
Table 1: Values for $S_i(i = 1, 2, \cdots, 7)$ for $\bar{n} = 10^4$ and $k = 2$. “Value1” denotes value of the resulting sums of the algorithm when we expand $f_{i1}(x, \bar{n}, k)$ to $x^{10}$ and “Value2” denotes that when we expand $f_{i1}(x, \bar{n}, k)$ to $x^{15}$. Value1 and Value2 are the same to the precision $10^{-23}$.

| Sum  | Value1               | Value2               |
|------|----------------------|----------------------|
| $S_1$ | 0.000 039 303 916 656 063 668 651 091 | 0.000 039 303 916 656 063 668 561 194 770 |
| $S_2$ | 0.000 039 265 164 255 300 772 996 074 590 | 0.000 039 265 164 255 300 772 995 750 283 |
| $S_3$ | 0.000 246 659 192 761 352 167 541 307 293 | 0.000 246 659 192 761 352 167 542 042 758 |
| $S_4$ | 0.999 753 309 972 685 637 856 777 333 369 | 0.999 753 309 972 685 637 856 776 237 858 |
| $S_5$ | 0.999 753 316 133 881 571 308 212 070 145 | 0.999 753 316 133 881 571 308 210 974 684 |
| $S_6$ | 0.999 753 322 301 165 250 291 025 614 276 | 0.999 753 322 301 165 250 291 024 518 866 |
| $S_7$ | 0.000 039 226 416 698 193 755 826 600 887 | 0.000 039 226 416 698 193 755 826 600 887 |

**Theorem 1:** For every given integer $l << \bar{n}$, let

$$p = \left\lfloor \frac{\ln \left( \sqrt{2\bar{n}}^{l-\frac{1}{2}(l+1)\ln \bar{n}} \right)}{\frac{1}{2} \ln \bar{n} - \ln \left( (l+1)\ln \bar{n} \right)} \right\rfloor,$$

(5)

$$\alpha_0 = \frac{1}{\sqrt{\bar{n}}} + \frac{(l+1) \ln \bar{n}}{\sqrt{\bar{n}}} + \frac{(l+1)^2 (\ln \bar{n})^2}{2\bar{n}} + 2(l+1) \ln \bar{n}.$$

If $\alpha_0 < \alpha << \sqrt{\bar{n}}$, then

$$\sum_{n=0}^{\infty} \frac{e^{-\bar{n}n}}{n!} f_{i0}(n, \bar{n}, k) = \sum_{n=0}^{\infty} \frac{e^{-\bar{n}n}}{n!} f_{i3}(n, \bar{n}, k) + o\left(\frac{1}{n!}\right),$$

(6)

here $p, f_{i0}(n, \bar{n}, k), f_{i3}(n, \bar{n}, k)$ are parameters defined in the algorithm above.

Theorem 1 can be proved using the following three lemmas (see Appendix A for the detailed proof):

**Lemma 1:** For every given $\alpha << \sqrt{\bar{n}},$

$$\sum_{n=\bar{n} - \alpha \sqrt{\bar{n}}}^{\bar{n} + \alpha \sqrt{\bar{n}}} \frac{e^{-\bar{n}n}}{n!} (f_{i0}(n, \bar{n}, k) - f_{i3}(n, \bar{n}, k)) = o\left(\frac{\alpha^{p+1}}{(\sqrt{\bar{n}})^{p+1}}\right),$$

(7)

here $p, f_{i0}(n, \bar{n}, k), f_{i3}(n, \bar{n}, k)$ are parameters defined in the algorithm above.

**Lemma 2:** For every given integer $l << \bar{n}, \alpha << \sqrt{\bar{n}},$ if $\alpha > \sqrt{(l+1)\ln \bar{n}},$ then

$$\sum_{n=0}^{k} \frac{e^{-\bar{n}n}}{n!} < \frac{1}{n!},$$

(8)

where $k = \left\lfloor \bar{n} + \alpha \sqrt{\bar{n}} \right\rfloor$.

**Lemma 3:** For every given integer $l << \bar{n}, \alpha << \sqrt{\bar{n}},$ if

$$\alpha > \frac{1}{\sqrt{\bar{n}}} + \frac{(l+1) \ln \bar{n}}{\sqrt{\bar{n}}} + \frac{(l+1)^2 (\ln \bar{n})^2}{2\bar{n}} + 2(l+1) \ln \bar{n},$$

(9)

then

$$\sum_{n=k}^{\infty} \frac{e^{-\bar{n}n}}{n!} < \frac{1}{n!},$$

(10)
where $k' = \lfloor \bar{n} + \alpha \sqrt{n} \rfloor$.

We expand $f_1(x, \bar{n}, k)$ to $x^{15}$ at $x = 0$, and find the value of the sum is the same to the precision $10^{-23}$ as that when we expand $f_1(x, \bar{n}, k)$ to $x^{10}$. It implies that the precision of the sum is much higher than Eq. (5) shows. The reason is probably that we have not considered of the periodicity of trigonometric functions, and the precision of the sum may be remarkably improved since the positive and negative terms will cancel each other out.

For small $\bar{n}$, we need only to require $t$ satisfying

$$(t - 1)! > e^{-\bar{n}} n^{t + l},$$

where $t$ is the parameter in sum $S_i(\bar{n}, k) = \sum_{n=0}^{t} \frac{e^{-\bar{n}} n^m}{n!} f_{i0}(n, \bar{n}, k) + o\left(\frac{1}{n}\right)$. For a given precision $l$, we can search out the smallest $t$ satisfying (11), e.g., when $\bar{n} = 10$ and $l = 20$, we get $t = 55$.

3. Population inversion

3.1. Final state of the two-level system after pulse train

Provided $r^{(m)} = Mr^{(m-1)} + c$, then

$$r^{(m)} = M^m r^{(0)} + (M^{m-1} + \cdots + M + I)c.$$  \hspace{1cm} (12)

It can be seen from Sec. 2.2 that

$$M^m = \begin{bmatrix} (S_3 + S_5)^m & 0 \\ O & M_1^m \end{bmatrix}, \quad M_1 = \begin{bmatrix} S_5 - S_3 & -(S_1 + S_7) \\ S_2 & S_4 + S_6 - 1 \end{bmatrix},$$

For any real matrix $A = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$, we obtain (see Appendix B)

$$A^m = \frac{\Lambda^+(m)}{2} I + \frac{\Lambda^-(m)}{2iQ} \begin{bmatrix} -K & 2b \\ 2c & K \end{bmatrix},$$

where $\Lambda^\pm(m) = \lambda_1^m \pm \lambda_2^m$ with $\lambda_1$ and $\lambda_2$ eigenvalues of $A$, $K = d - a$, $Q = -i \sqrt{(a - d)^2 + 4bc}$. When $(a - d)^2 + 4bc < 0$ (which is the case for $M_1$)

$$A^m = |\lambda|^m \left[ \cos(m\theta) I + \sin(m\theta) \frac{J}{\sqrt{\det J}} \right],$$

where $|\lambda|^2 = ad - bc$, $\sin \theta = \frac{1}{2} \sqrt{2 - \frac{a^2 + d^2 + 2bc}{ad - bc}}$, $J = \begin{bmatrix} a - d & 2b \\ 2c & d - a \end{bmatrix}$. Therefore,

$$I + M_1 + \cdots + M_1^{m-1} = \left[ \sum_{j=0}^{m-1} |\lambda|^j \cos(j\theta) \right] I + \left[ \sum_{j=0}^{m-1} |\lambda|^j \sin(j\theta) \right] \frac{J}{\sqrt{\det J}}.$$
Since
\[
\sum_{j=0}^{m-1} \{ |\lambda|^j [\cos(j\theta) + i \sin(j\theta)] \} = \sum_{j=0}^{m-1} (|\lambda|^j e^{i(j\theta)}) = \sum_{j=0}^{m-1} (|\lambda|e^{i\theta})^j
\]
\[
= \frac{1 - |\lambda|e^{-i\theta} - |\lambda|^m e^{i(m\theta)} + |\lambda|^{m+1}e^{i(m-1)\theta}}{1 + |\lambda|^2 - 2|\lambda| \cos \theta},
\]
we have
\[
\sum_{j=0}^{m-1} |\lambda|^j \cos(j\theta) = \frac{1 - |\lambda| \cos \theta - |\lambda|^m \cos(m\theta) + |\lambda|^{m+1} \cos(m - 1)\theta}{1 + |\lambda|^2 - 2|\lambda| \cos \theta},
\]
\[
\sum_{j=0}^{m-1} |\lambda|^j \sin(j\theta) = \frac{|\lambda| \sin \theta - |\lambda|^m \sin(m\theta) + |\lambda|^{m+1} \sin(m - 1)\theta}{1 + |\lambda|^2 - 2|\lambda| \cos \theta},
\]
thus
\[
I + M_1 + \cdots + M_1^{m-1}
\]
\[
= \frac{1}{1 + |\lambda|^2 - 2|\lambda| \cos \theta} \left[ (1 - |\lambda| \cos \theta - |\lambda|^m \cos(m\theta) + |\lambda|^{m+1} \cos(m - 1)\theta) I
\]
\[
+ ( |\lambda| \sin \theta - |\lambda|^m \sin(m\theta) + |\lambda|^{m+1} \sin(m - 1)\theta) \frac{J}{\sqrt{\det J}} \right]
\]
\[
\triangleq B_1^{(m)} I + B_2^{(m)} J,
\]
then
\[
r^{(m)} = \begin{bmatrix} (S_3 + S_5)^m & 0 \\ O & |\lambda|^{\frac{m}{2}} \left[ \cos(m\theta) I + \sin(m\theta) \frac{J}{\sqrt{\det J}} \right] \end{bmatrix} r^{(0)}
\]
\[
+ \begin{bmatrix} \frac{1 - (S_3 + S_5)^m}{1 - S_3 - S_5} & 0 \\ O & B_1^{(m)} I + B_2^{(m)} J \end{bmatrix} c.
\]

3.2. Population inversion after pulse train

Suppose the initial state is |1⟩, if we have applied \( k \pi \) pulses for \( m \) times, the population inversion is
\[
W_m = \frac{1}{2} (1 - r_z^{(m)}) - \frac{1}{2} (1 + r_z^{(m)}) = -r_z^{(m)},
\]
we have
\[
W_m = |\lambda|^m \left[ \cos(m\theta) + \sin(m\theta) \frac{\dot{j}_{22}}{\sqrt{\det J}} \right] - \frac{1}{1 + |\lambda|^2 - 2|\lambda| \cos \theta}
\]
\[
\times \left\{ \left[ |\lambda| \sin \theta - |\lambda|^m \sin(m\theta) + |\lambda|^{m+1} \sin(m - 1)\theta \right] \frac{\dot{j}_{21}}{\sqrt{\det J}} (S_7 - S_1)
\]
\[
+ \left[ (1 - |\lambda| \cos \theta - |\lambda|^m \cos(m\theta) + |\lambda|^{m+1} \cos(m - 1)\theta) \right] \frac{\dot{j}_{22}}{\sqrt{\det J}} (S_4 - S_6) \right\}.
\]
To get the inversion between the \( m \)th and \((m + 1)\)th \( \pi \) pulse, we should first get the corresponding density matrix of the two-level system

\[
\rho_n(t) = \text{tr} \left\{ U(t) [\rho^{(m)} \otimes \rho] U^\dagger(t) \right\},
\]

where \( U(t) \) is the unitary time-evolution operator mentioned earlier, and \( \rho \) is the density matrix for the laser field. A detailed calculation gives the probability that the ion is in state \( |0\rangle \):

\[
p(t) = \frac{1}{2} \left[ (S_S + S_0) + r_x^{(m)}(t)(S_S - S_0) + r_y^{(m)}(t) S_{10} \right],
\]

where

\[
S_S = \sum_{n=0}^{\infty} \frac{e^{-n \bar{n}}}{n!} \cos^2 \sqrt{n}, \quad S_0 = \sum_{n=0}^{\infty} \frac{e^{-n \bar{n}}}{n!} \sin^2 \sqrt{n} + 1, \quad S_{10} = \sum_{n=0}^{\infty} \frac{e^{-n \bar{n}}}{n!} \sqrt{\pi} \sin 2gt \sqrt{n},
\]

which can all be got with high precision using our algorithm in Section 2.3, and the inversion is \( W_m(t) = 1 - 2p(t), 0 < t < \frac{k\pi}{2\sqrt{\bar{n}}} \).

Now think of the difference of the oscillation driven by pulse train and a cw field. The population inversion for repeated \( 2\pi \) pulses is shown in Figure 1a (given \( \bar{n} = 10 \)). We find there is a dual-pulse structure in every period, where the amplitude starts to increase from the point of \( 2\pi \) pulses. The inversion decreases exponentially, different from a Gaussian function collapse envelope driven by a cw field. Besides, there is no revival phenomenon, but a small nonzero amplitude exists. The reason for this behavior is probably that the system we consider here is an open quantum system with dissipation.

The inversion at the points of \( 2\pi \) pulses when \( \bar{n} = 10^4 \) is plotted in Figure 2. Results of fitting is \( 1.0031e^{-0.0002N_R}, 1.0193e^{-0.0003N_R}, 1.025e^{-0.0005N_R} \) for \( k = 1/2, 1, 2 \) respectively, here \( N_R \) is the number of Rabi periods.

4. Failure probability of gate operation realized through Rabi oscillation driven by repeated pulses

4.1. Estimation of \( \bar{n} \)

\( \bar{n} \) which determines \( S_i \) is an important parameter in our discussion. To estimate the mean number of photons in one pulse, we assume a fictious pulse propagating in the opposite direction at the same time. They form a standing wave instantly while overlapping in space. It can be seen that the mean number of photons in each pulse is about half of that in the standing wave. We now focus on mean number of photons in the imagined standing wave.

The electric field \( E \) can be expressed as \( E = \mathcal{E} \sqrt{\bar{n}} \). \( \mathcal{E} \) is usually given as \( \mathcal{E} = \frac{\hbar \omega}{e a_0} \sqrt{V} \) [20], where \( \omega \) is the frequency of the single mode in a cavity, and \( V \) is the volume of the cavity. It can be seen that \( V \sim Act \), with \( A \) the cross-sectional area of the beam, thus

\[
\bar{n} = \frac{\omega A \hbar c t}{e a_0} E^2.
\]

For a \( k\pi \) pulse, \( gt \sqrt{\bar{n}} = \frac{k\pi}{2} \), \( g \sim \frac{\mathcal{E}}{\bar{n}} = \frac{p E}{k \sqrt{\bar{n}}} \), with \( p \sim e a_0 \) the electric dipole moment of the ion, \( e \) the charge of an electron, and \( a_0 \) Bohr radius, then we get \( t = \frac{k\pi \hbar}{2pE} \). Then we have \( \bar{n} = \frac{k\pi \hbar}{2pE} \).

When the laser beam interacts with an ion, not all the photon in the beam are effective. Think of the effective mean number of photons. When a laser beam is
Figure 1: Population inversion driven by different fields, given $\bar{n} = 10$, $\tau = gt$. (a) $2\pi$ pulse train case. There is a dual-pulse structure in every period, where the amplitude starts to increase from the point of $2\pi$ pulses. The inversion decreases exponentially, different from a Gaussian function collapse envelope driven by a cw field. Besides, there is no revival phenomenon, but a small nonzero amplitude exists. (b) Corresponding inversion driven by a cw field.

applied to a trapped ion, the total resonant scattering cross section for an atomic dipole transition is $\sigma = 3\lambda^2/2\pi$ [21], and the cross section for scattering out of the paraxial modes is $\sigma_{eff} = 3\lambda^2/8\pi$ [22]. Then the effective interaction area is $\sigma_{eff}$, and the photons in volume $\sigma_{eff}ct$ is effective. For each photon, the probability to be in area $\sigma_{eff}$ is $\frac{\sigma_{eff}}{A}$, and the probability are independent for the photons. It can be seen that the effective
Figure 2: Inversion at the points of $2\pi$ pulses $E(W)$ versus number of Rabi periods $N_R$, $\bar{n} = 10^4$. Fitting results are $1.0031e^{-0.0002N_R}$, $1.0193e^{-0.0003N_R}$, $1.025e^{-0.0005N_R}$ for $k = \frac{1}{2}, 1, 2$ respectively.

mean number of photons is

$$\bar{n}_{\text{eff}} = \frac{\bar{n}}{\sigma_{\text{eff}}} = \frac{k}{4} \frac{\epsilon_0 \sigma_{\text{eff}} \lambda}{p} E.$$  \hspace{1cm} (16)

One case people are interested in is the sideband transition, where the laser detuning $\Delta = \pm \omega_i$, here $\omega_i$ is the frequency of the trap. Because of AC-Stark shift and off-resonant transitions, the sideband Rabi frequency $\Omega_+$ has upper bound [23]. People have adopted methods to partially cancel the effect, and it seems feasible to have $\Omega_+ < \omega_i$ for special temporal and spectral arrangements of the laser field [24]. Since $\Omega_+ = \frac{2\pi}{\lambda} \sqrt{\frac{\hbar}{2M \omega_i}} \Omega$, with $M$ the mass for a single ion, we have

$$\Omega < \frac{\lambda}{2\pi} \sqrt{\frac{2M}{\hbar}} \frac{4}{\omega_i^2}. \hspace{1cm} (17)$$

From [25] and [26], it can be seen that

$$\Omega = \frac{e a_0 E}{4 \hbar} = \frac{p E}{4 \hbar},$$

$$\omega_i = \sqrt{\frac{e^2}{4 \pi \epsilon_0 M z_s^3}}, \hspace{1cm} (18)$$

where $z_s$ is the order of the separation between ions and is typically 10 to 100 $\mu$m. Suppose $z_s = \xi \lambda$, from (17) and (18), we get

$$E < \frac{2\sqrt{2\hbar}}{p \pi} (\frac{e^2}{4 \pi \epsilon_0})^{\frac{1}{4}} \frac{M^{-\frac{1}{4}} \xi^{-\frac{3}{4}} \lambda^{-\frac{7}{4}}}{h}. \hspace{1cm} (19)$$

Substitute back to (16), we get

$$\bar{n} < \frac{3 \xi_0^{\frac{1}{4}}}{32 a_0^2 \pi^{\frac{1}{4}}} \sqrt{\frac{h}{e}} k M^{-\frac{1}{4}} \xi^{-\frac{9}{4}} \lambda^{\frac{7}{4}}$$

$$= 6 \times 10^7 k M^{-\frac{1}{4}} \xi^{-\frac{9}{4}} \lambda^{\frac{7}{4}}. \hspace{1cm} (20)$$
In the cases we consider, it is suitable to limit $k \leq 2$, $9u \leq M \leq 200u$ ($u = 1.66057 \times 10^{-27}$ kg). For $M = 9u$, $k = 2$, we get

$$\bar{n} = 3.4 \times 10^{14} \xi^{-\frac{2}{7}} \lambda^{2}.$$ 

We can see that a large $\lambda$ and a small $\xi$ result in a large $\bar{n}$. The curves of $\log(\bar{n})$ is plotted in Figure 3 versus parameter $\xi$ from 2 to 100. When $\lambda = 10^{-6}$ m and $\xi = 2$, we get $\bar{n} = 2.3 \times 10^{3}$.

Figure 3: Logarithm of mean number of photons $\log(\bar{n})$ as a function of $\xi$ and $\lambda$. It can be seen that $\bar{n}$ increases with $\lambda$ and decreases with $\xi$.

There are also authors calculating $\bar{n}$ in a $k\pi$ pulse in another way [15]: they considered the situation where a single laser is used to drive Rabi oscillation of the atom, and adopted the formalism introduced by Blow et al. [27], taking the laser as a continuous-mode coherent state. They worked out the interaction time $t$ for $k\pi$ pulse as $t = \frac{k\pi}{d} \sqrt{\frac{\omega c A}{2P}}$, where $d$ is the coupling constant of the atom and laser, and $P$ is the power of the laser. Thus, the mean number of photons in one $k\pi$ pulse is

$$\bar{n} \approx \frac{Pt}{\hbar \omega_L} = \frac{k\pi}{\omega_L d} \sqrt{\frac{\omega c A P}{2}},$$

where $\omega_L$ is the frequency of the representative single-mode coherent state. Thus, obviously, they take all the photons in area $A$ as effective photons when considering the interaction, but actually the number of effective photons is much smaller.

4.2. Accuracy of gate operation

Suppose we have applied $m$ times of coherent pulses and reached a state $\rho^{(m)} = \frac{1}{2}(I + r^{(m)} \cdot \sigma)$. Let $|\Psi\rangle = \alpha |0\rangle + \beta |1\rangle$ be the expected state, the accuracy rate of gate operation realized through Rabi oscillation is

$$p_{s}^{(m)} = (\alpha^{*} |0\rangle + \beta^{*} |1\rangle) \rho^{(m)} (\alpha |0\rangle + \beta |1\rangle)$$

$$= |\alpha|^{2} \rho_{11}^{(m)} + |\beta|^{2} \rho_{22}^{(m)} + \alpha^{*} \beta \rho_{12}^{(m)} + \alpha \beta^{*} \rho_{21}^{(m)}$$

$$= \frac{1}{2} \left(1 + r_{x}^{(0)} r_{x}^{(m)} + r_{y}^{(0)} r_{y}^{(m)} + r_{z}^{(0)} r_{z}^{(m)}\right)$$

$$= \frac{1}{2} (1 + r^{(0)} \cdot r^{(m)}),$$

(21)
for a mixed state, $|r^{(m)}| < 1$, then $p_s < 1$. The failure probability is $p_f^{(m)} = 1 - p_s^{(m)}$. A detailed calculation results (see Appendix C)

$$p_f^{(m)} = -\frac{1}{2}(r^{(0)} \cdot r^{(m)} - 1)$$

$$= -\frac{1}{2}\left\{(r_x^{(0)})^2[(S_3 + S_5)^m - 1] + ((r_y^{(0)})^2 + (r_z^{(0)})^2)[|\lambda|^\frac{m}{2} \cos(m\theta) - 1]ight.$$ 
$$+ |\lambda|^\frac{m}{2} \sin(m\theta)(\det J)^{-\frac{1}{2}}[((r_y^{(0)})^2 - (r_z^{(0)})^2)(a - d) + r_y^{(0)}r_z^{(0)}(b + c)]$$
$$+ B_1^{(m)}(r_y^{(0)}c_y + r_z^{(0)}c_z) + B_2^{(m)}[(r_y^{(0)}c_y - r_z^{(0)}c_z)(a - d) + r_z^{(0)}c_y c + r_y^{(0)}c_z b]\right\}. $$

Then we average over all initial states of the ion, and get the average failure probability. The failure probability for $k\pi$ pulses with different $\bar{n}$ are shown in Figure 4. It can be seen that the failure probability increases with the number of Rabi periods $N_R$ and the value $k$, and is inversely proportional to $\bar{n}$.

Figure 4: Failure probability $p_f$ versus number of Rabi periods $N_R$, $k\pi$ pulses are applied, and $\bar{n}$ is $10^4$ ($10^6$) in a (b). The failure probability $p_f$ increases with the number of Rabi periods $N_R$ and the value $k$, and is inversely proportional to $\bar{n}$.

5. Discussions

5.1. The reason for tracing out the laser field after each pulse

For the Cirac-Zoller CNOT scheme, there are five steps to implement it. The laser phase in the five steps are $\pi/2, 0, 0, 0$ and $-\pi/2$, which are correlated. However, there is no correlation between two different CNOT gates. Then after completing one CNOT gate, it is valid to trace out the laser field. The calculation in Sec. 2 for different pulses is an analog of different CNOT gates. This treatment is meaningful for our purpose, i.e., to estimate the lower bound of failure probability, or the upper bound of operation
number, after many CNOT operations. More-detailed analysis of the lower bound of failure probability after Cirac-Zoller CNOT operations can be seen in [28], and the main idea of [28] is summarized in Appendix D.

5.2. The permitted depth of quantum logical operation

Failure probability we have calculated for the $\pi$ sideband transition amounts to $10^{-2}$ after approximately $10^2$ operations when $\bar{n} = 10^4$. For controlled-NOT (CNOT) gates, there are five steps in Cirac-Zoller scheme, and two steps are realized via Rabi oscillations driven by $\pi$ pulses. Generally speaking, the failure probability after five steps is not less than that after one $\pi$ pulse. Then the failure probability after repeated $\pi$ pulses is a lower bound of the failure probability after repeated Cirac-Zoller’s CNOT gate. Thus the lower bound of the failure probability is $10^{-2}$ after approximately $10^2$ CNOT operations when $\bar{n} = 10^4$.

The threshold theorem in quantum computation declares that an arbitrarily long quantum computation can be performed reliably if the failure probability of each quantum gate is less than a critical value. Knill used numerical calculations and obtained a threshold of the order $10^{-2}$ [29] based on a fault-tolerant structure suggested by himself. P. Aliferis et al. reached a threshold of $10^{-3}$ with provable constructions [30].

A parameter called permitted depth of logical operation describing the property of a physical realization scheme of QC has been given [9]: considering that different number state components of the driving field lead to different oscillation amplitudes, which become uncorrelated gradually, we can see that failure probability of quantum logic gates has a theoretical limitation. Combing this limitation given by the quantum nature of the field with the threshold theorem in FTQC, we can get permitted depth of logical operation. This parameter limits the number of operations on any physical qubit in one error-correction period. Then the permitted depth of logical operation here is less than $10^2$.

5.3. Others’ proposals which may have different results

For Rabi oscillation driven by microwaves, the failure probability may be much smaller because of a large mean number of photons, but it becomes difficult to individually address each ions. Although an additional magnetic field gradient applied to an electrodynamic trap may individually shift ionic qubit resonances [31], thus making them distinguishable in frequency space, whether it can improve the permitted depth of logical operation needs further investigation.

There exists a two-qubit gate scheme totally different from the Cirac-Zoller gate, such as the scheme implemented by the NIST group [32]. In the scheme off-resonant excitations of the stronger carrier transition is absent, and this allows a greater gate speed thus a higher laser intensity. Besides, additional Stark shifts can be efficiently suppressed by choosing almost perpendicular and linear polarizations for the laser beams [33]. Hence, studies on this type of gate may lead to different results.
6. Conclusions

Firstly, we investigate Rabi oscillation of a two-level system driven by pulse train. We develop an algorithm to solve the infinite summation, with a high precision which has never been reached by former authors. We find that in this kind of Rabi oscillation, there is a dual-pulse structure in every period. The envelope of population inversion collapses exponentially, different from a Gaussian function collapse envelope driven by a cw field. Besides, there is no revival phenomenon, but an approaching to a tiny platform.

Secondly, we consider the application to gate operation in ion trap quantum computation. We give a lower bound of failure probability. Our result is: that when the wavelength of the driving field is of the order $10^{-6}$ m, the mean number of photons cannot be greater than $10^4$. Then, after about $10^2$ CNOT gates in Cirac-Zoller scheme, the lower bound of failure probability is of the order $10^{-2}$.

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Appendix A. PROOF OF PRECISION OF THE ALGORITHM IN SEC. 2.3

Proof of Lemma 1: For $\bar{n} - \alpha \sqrt{n} < n < \bar{n} + \alpha \sqrt{n}$, i.e. $-\alpha \sqrt{n} < x < \alpha \sqrt{n}$, after expanding $f_{i1}(x, \bar{n}, k)$ at $x = 0$, we get the result $f_{i2}(x, \bar{n}, k)$ satisfying $f_{i2}(x, \bar{n}, k) = f_{i0}(\bar{n}, \bar{n}, k) + o(x^p)$. It can be seen that $f_{i2}(x, \bar{n}, k) = f_{i3}(n, \bar{n}, k)$, thus we have

$$f_{i0}(n, \bar{n}, k) = f_{i3}(n, \bar{n}, k) + o(x^p),$$

then Eq. (7) is proved.

Proof of Lemma 2: For every given $n$ satisfying $n < k + 1 < \bar{n}$, we have

$$\frac{n^k}{k!} < \frac{(\bar{n})^{k+1}}{(k+1)!},$$

From Stirling’s formula $k! = \sqrt{2\pi k}(\frac{k}{e})^k e^{\theta_1}$, $0 < \theta < 1$, we have

$$e^{-\bar{n}} \frac{n^{k+1}}{k!} < \frac{e^{\bar{n}}}{k} e^{-\bar{n}} \frac{n^{k+1}}{(k+1)!} = e^{k-\bar{n}} \frac{\bar{n}^{k-1}}{k}. \quad (A.1)$$

Substitute $k$ in formula (A.2) with $n - \alpha \sqrt{n}$, we have

$$e^{k-\bar{n}} \frac{\bar{n}^{k-1}}{k} = \bar{n} e^{-\alpha \sqrt{n}} (1 - \frac{\alpha}{\sqrt{n}})^{-\frac{n}{\bar{n}}} (\alpha \sqrt{n} - \alpha^2) \bar{n} e^{-\alpha \sqrt{n}} e^{\alpha \sqrt{n} - \alpha^2} = \bar{n} e^{-\alpha^2}.$$

When $\alpha > \sqrt{(l + 1) \ln \bar{n}}$, we have $\bar{n} e^{-\alpha^2} < \frac{1}{\bar{n}}$, inequality (8) is proved.
Proof of Lemma 3: It can be seen that
\[ \sum_{n=k'}^{\infty} e^{-\bar{n}^{k'}} n! = \frac{e^{-\bar{n}^{k'}}}{k'+1} \sum_{n=k'}^{\infty} \frac{\bar{n}^{n-k'}k'}{n!} \]
when \( k' > \bar{n} + \frac{1}{\bar{n}} \), i.e., \( \frac{k'+\frac{1}{\bar{n}}}{k'+1} < k' \), we have
\[ e^{-\bar{n}^{k'}} \frac{k'+1}{k'}! < \left( \frac{e}{k'} \right)^{k'} e^{-\bar{n}^{k'+1}} < \bar{n} e^{-\bar{n}^{k'}} \frac{(k'-1)!}{(k'-1)!} \]
with Stirling’s formula we get
\[ \left( \frac{e}{k'} \right)^{k'} e^{-\bar{n}^{k'}} \frac{(k'-1)!}{(k'-1)!} < \bar{n} e^{-\bar{n}^{k'}} \frac{(k'-1)!}{(k'-1)!} = \bar{n} e^{-\bar{n}^{k'-1}} \]
Let \( \lambda = \frac{\bar{n}}{k'-1} < 1, \eta = \bar{n} \frac{1}{k'+1} \), we then have
\[ \bar{n} e^{-\bar{n}^{k'-1}} = \bar{n} e^{-\bar{n}^{k'}} < \frac{1}{\bar{n}!} \iff \left( \frac{\bar{n}}{k'-1} \right)^{k'-1} < \frac{e^{\bar{n}}}{\bar{n}+1} \iff \frac{\bar{n}}{\eta} - \lambda \eta > 0 \]
\[ \iff \lambda(1 - \ln \eta) > 1 + \ln \lambda. \]
Let \( \lambda = 1 - \Delta, 0 < \Delta < 1 \), from \( \ln(1+x) < x - \frac{1}{2}x^2 \) \((x < 0)\), we get \( \ln \lambda < -\Delta - \frac{1}{2} \Delta^2 \),
then a sufficient condition of \( \left( \frac{\eta}{\eta} \right)^{\lambda} - \lambda \eta > 0 \) is:
\[ (1 - \Delta)(1 - \ln \eta) > 1 - \Delta - \frac{1}{2} \Delta^2, \]
which results in \( \Delta > \Delta_0 \), here \( \Delta_0 \equiv -\ln \eta + \sqrt{(\ln \eta)^2 + 2 \ln \eta} \). Let \( \frac{\bar{n}}{k+1} = \bar{n} + \alpha_0 \sqrt{\bar{n}} \), we get
\[ \alpha_0 = \frac{1}{\sqrt{\bar{n}}} \left[ \left( \frac{1}{1 - \Delta_0} - 1 \right) \bar{n} + 1 \right] \]
\[ = \frac{1}{\sqrt{\bar{n}}} + \left( \frac{l+1}{\bar{n}} \ln \bar{n} + \sqrt{\left( \frac{l+1}{\bar{n}} \ln \bar{n} \right)^2 + \frac{2(l+1)}{\bar{n}} \ln \bar{n}} \right) \sqrt{\bar{n}} \]
by using \( \frac{1}{1 - \Delta_0} = 1 + \ln \eta + \sqrt{(\ln \eta)^2 + 2 \ln \eta} \) and \( \eta = \left( \frac{n}{\bar{n}} \right)^{\frac{l+1}{\bar{n}}} \). Because \( \Delta > \Delta_0 \iff \alpha > \alpha_0 \),
we get a sufficient condition of Lemma 3:
\[ \alpha > \frac{1}{\sqrt{\bar{n}}} + \left( \frac{l+1}{\bar{n}} \ln \bar{n} + \sqrt{\left( \frac{l+1}{\bar{n}} \ln \bar{n} \right)^2 + \frac{2(l+1)}{\bar{n}} \ln \bar{n}} \right) \sqrt{\bar{n}} \]
\[ = \frac{1}{\sqrt{\bar{n}}} + \left( \frac{l+1}{\bar{n}} \ln \bar{n} + \sqrt{\left( \frac{(l+1)^2}{\bar{n}} \ln \bar{n}^2 \right)^2 + 2(l+1) \ln \bar{n}} \right) \sqrt{\bar{n}} \]
then Lemma 3 follows. \( \square \)

Proof of Theorem 1: From Lemma 1, 2 and 3 we get: for every given \( l << \bar{n} \),
if \( \alpha \) satisfies
\[
\frac{1}{\sqrt{n}} + \frac{(l + 1) \ln \bar{n}}{\sqrt{n}} + \sqrt{\frac{(l + 1)^2 (\ln \bar{n})^2}{\bar{n}}} + 2(l + 1) \ln \bar{n} < \alpha << \sqrt{n},
\]

(A.3)

(7), (8) and (10) hold. Then

\[
S_i = \sum_{n=0}^{\infty} e^{-\bar{n} n^m} f_{i0}(n, \bar{n})
\]

= \sum_{n=0}^{\infty} \frac{e^{-\bar{n} n^m}}{n!} (f_{i0}(n, \bar{n}) - f_{i3}(n, \bar{n}))

+ \sum_{n=\bar{n} + \alpha \sqrt{n}}^{\infty} \frac{e^{-\bar{n} n^m}}{n!} (f_{i0}(n, \bar{n}) - f_{i3}(n, \bar{n}))

+ \sum_{n=\bar{n} - \alpha \sqrt{n}}^{\infty} \frac{e^{-\bar{n} n^m}}{n!} (f_{i0}(n, \bar{n}) - f_{i3}(n, \bar{n}, k))

= \sum_{n=0}^{\infty} \frac{e^{-\bar{n} n^m}}{n!} f_{i3}(n, \bar{n}, k) + o\left(\frac{1}{n^l}\right) + o\left(\frac{\alpha^{p+1}}{(\sqrt{n})^{p-1}}\right).
\]

Let \(o\left(\frac{1}{n^l}\right) = o\left(\frac{\alpha^{p+1}}{(\sqrt{n})^{p-1}}\right)\), we get

\[
p = \left\lfloor \ln \left(\frac{\sqrt{2} n^l + \frac{1}{2} (l + 1) \ln \bar{n}}{\ln \bar{n} - \ln ((l + 1) \ln \bar{n})}\right) \right\rfloor,
\]

then \(S_i = \sum_{n=0}^{\infty} \frac{e^{-\bar{n} n^m}}{n!} f_{i3}(n, \bar{n}) + o\left(\frac{1}{n^l}\right)\). Since we can get exact result of \(\sum_{n=0}^{\infty} \frac{e^{-\bar{n} n^m}}{n!} f_{i3}(n, \bar{n})\), we get \(S_i\) with precision \(o\left(\frac{1}{n^l}\right)\). \(\square\)

Appendix B. CALCULATION OF \(M_1^m\)

Let

\[
M = \begin{bmatrix} S_3 + S_5 & 0 \\ O & M_1 \end{bmatrix},
\]

where

\[
M_1 = \begin{bmatrix} S_5 - S_3 & -(S_1 + S_7) \\ S_2 & S_4 + S_6 - 1 \end{bmatrix} \triangleq \begin{bmatrix} a & b \\ c & d \end{bmatrix},
\]

then

\[
M^m = \begin{bmatrix} (S_3 + S_5)^m & 0 \\ O & M_1^m \end{bmatrix}.
\]
Figure B1: $\Delta(\tau) = (a - d)^2 + 4bc < 0$ versus $\tau = gt$, where $t$ is the pulse width. Different $\Delta(\tau)$ results in different behavior of Rabi oscillation driven by pulse train. For the cases we consider, $\tau < 1$, we can see $\Delta(\tau) < 0$.

Let $(1, x_{21})^T$ and $(1, x_{22})^T$ be the eigenvectors of $M_1$ with corresponding eigenvalues $\lambda_1$ and $\lambda_2$, then

\[
x_{21} = \frac{1}{2b} \left[ d - a + \sqrt{(a - d)^2 + 4bc} \right],
\]
\[
x_{22} = \frac{1}{2b} \left[ d - a - \sqrt{(a - d)^2 + 4bc} \right],
\]
\[
\lambda_1 = \frac{1}{2} [a + d + \sqrt{(a - d)^2 + 4bc}],
\]
\[
\lambda_2 = \frac{1}{2} [a + d - \sqrt{(a - d)^2 + 4bc}],
\]

we have plot $\Delta(\tau) = (a - d)^2 + 4bc$ versus $\tau = gt$ in Figure B1. $\Delta(\tau)$ is below zero for the cases we are interested in ($\tau < 1$).

Let

\[
T_1 = \begin{bmatrix} 1 & 1 \\ x_{21} & x_{22} \end{bmatrix},
\]

thus

\[
M_1 = T_1 \begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix} T_1^{-1},
\]

then,

\[
M_1^m = T_1 \begin{bmatrix} \lambda_1^m & 0 \\ 0 & \lambda_2^m \end{bmatrix} T_1^{-1} = \frac{1}{x_{21} - x_{22}} \begin{bmatrix} -x_{22} \lambda_1^m + x_{21} \lambda_2^m & \lambda_1^m - \lambda_2^m \\ x_{21} x_{22} (-\lambda_1^m + \lambda_2^m) & x_{21} \lambda_1^m - x_{22} \lambda_2^m \end{bmatrix}.
\]

Denote $\lambda_1^m \pm \lambda_2^m = \Lambda_{\pm}^{(m)}$, $d - a = K$, $\sqrt{(a - d)^2 + 4bc} = iQ$, we have

\[
M_1^m = \frac{\Lambda^m}{2} I + \frac{\Lambda^{(m)}}{2iQ} \begin{bmatrix} -K & 2b \\ 2c & K \end{bmatrix}.
\]

It can be seen that $|\lambda_1| = |\lambda_2|$, let $\lambda_1 = |\lambda| e^{i\theta}$, $\lambda_2 = |\lambda| e^{-i\theta}$, using $|\lambda|^2 = \lambda_1 \lambda_2 = ad - bc$, we get

\[
\Lambda_{\pm}^{(m)} = 2(ad - bc)^{m/2} \cos(m\theta),
\]
\[
\Lambda_{-}^{(m)} = 2i(ad - bc)^{m/2} \sin(m\theta),
\]
where \( \theta \) satisfies \( \sin \theta = \sqrt{\frac{2ad - 4bc - a^2 - d^2}{4(ad - bc)}} \), then
\[
M_1^m = |\lambda|^m \left[ \cos(m\theta) I + \sin(m\theta) \frac{J}{\sqrt{\det J}} \right],
\]
where
\[
J = \begin{bmatrix}
a - d & 2b \\
2c & d - a
\end{bmatrix}.
\]

Appendix C. Calculation of \( r^{(0)} \cdot r^{(m)} \)

It can be seen from (12), (14), (B.1), (B.2) that
\[
r^{(0)} \cdot r^{(m)} = (r^{(0)})^T M^m r^{(0)} + (r^{(0)})^T \left[ \sum_{k=0}^{m-1} (S_3 + S_5)^k \frac{M_k}{O} \sum_{k=0}^{m-1} M_1^k \right]^c
\]
\[
= (r^{(0)})^T \left[ \frac{(S_3 + S_5)^m}{O} \right] r^{(0)} + (r^{(0)})^T \left[ \frac{1 - (S_3 + S_5)^m}{O} B_1^{(m)} I + B_2^{(m)} J \right]^c
\]
\[
= (r_x^{(0)})^2 (S_3 + S_5)^m + B_1^{(m)}(r_y^{(0)} c_y + r_z^{(0)} c_z) + ((r_y^{(0)})^2 + (r_z^{(0)})^2)|\lambda|^m \sin(m\theta)
\]
\[
+ |\lambda|^m \sin(m\theta) \frac{J}{\sqrt{\det J}} \begin{bmatrix} r_y^{(0)} & r_z^{(0)} \end{bmatrix} J \begin{bmatrix} r_y^{(0)} & r_z^{(0)} \end{bmatrix} + B_2^{(m)} \begin{bmatrix} r_y^{(0)} & r_z^{(0)} \end{bmatrix} J \begin{bmatrix} c_y^{(0)} & c_z^{(0)} \end{bmatrix}. \quad (C.1)
\]

Using
\[
\begin{bmatrix} r_y^{(0)} & r_z^{(0)} \end{bmatrix} J \begin{bmatrix} c_y^{(0)} \\ c_z^{(0)} \end{bmatrix} = (r_y^{(0)} c_y - r_z^{(0)} c_z)(a - d) + r_z^{(0)} c_y c + r_y^{(0)} c_z b,
\]
and
\[
\begin{bmatrix} r_y^{(0)} & r_z^{(0)} \end{bmatrix} J \begin{bmatrix} r_y^{(0)} \\ r_z^{(0)} \end{bmatrix} = ((r_y^{(0)})^2 - (r_z^{(0)})^2)(a - d) + r_y^{(0)} r_z^{(0)} (b + c),
\]
we get
\[
r^{(0)} \cdot r^{(m)} = (r_x^{(0)})^2 [(S_3 + S_5)^m - 1] + ((r_y^{(0)})^2 + (r_z^{(0)})^2)[|\lambda|^m \sin(m\theta) - 1]
\]
\[
+ |\lambda|^m \sin(m\theta) \frac{J}{\sqrt{\det J}} \left[ ((r_y^{(0)})^2 - (r_z^{(0)})^2)(a - d) + r_y^{(0)} r_z^{(0)} (b + c) \right]
\]
\[
+ B_1^{(m)}(r_y^{(0)} c_y + r_z^{(0)} c_z) + B_2^{(m)}[(r_y^{(0)} c_y - r_z^{(0)} c_z)(a - d) + r_z^{(0)} c_y c + r_y^{(0)} c_z b] + 1.
\]

Appendix D. More-detailed calculation for CNOT gate

Now, we consider the full-quantized treatment of Cirac-Zoller CNOT gate. The main idea is as follows: in the Cirac-Zoller scheme, the qubits are trapped ions and the phonon of the ion string’s collective motion. For the CNOT gate, suppose \( x \)th ion is the control qubit, and the \( y \)th ion is the target qubit. Then the initial state \( |\psi^{(0)}\rangle \) of the qubits (including \( x \)th ion, \( y \)th ion and the phonon) is a superposition of 12 computational basis states. Let the coefficients for the computational basis states be \( \alpha_i (i = 1, \cdots, 12) \). For each step of CNOT gate, full-quantized treatment is applied, and the laser field is not
traced out. Finally we get the state after one CNOT gate. Then we trace out the laser field, and get the density matrix of the ions and phonon after one CNOT gate. It has 144 elements, and the simplest element is
\[
\rho_{11}^{(1)} = a_1^* \left[ a_1 S_2^* S_4^* - a_3 S_3^* S_4^* + a_3 S_4^* S_3^* + a_1 S_1 S_3 - a_3 S_6^* S_10 + a_3 S_7^* S_4 + a_1 S_2 S_4 + a_1 S_5 S_10 \right] \\
+ a_3^* \left[ a_3 S_10 S_1 + a_1 S_1 S_2 - a_3 S_9^* S_4 - a_3 S_3^* S_8 - a_1 S_3 S_4 - a_1 S_6 S_10 + S_1(-a_3 S_3 + a_1 S_7) + a_3 S_8 S_10 \right],
\]
where \( S_i (i = 1, \cdots, 10) \) are sums with the form \( \sum_{n=0}^{\infty} \frac{e^{-\bar{n} n}}{n!} f(n, \bar{n}) \), with \( \bar{n} \) the mean number of photons in the pulse. The sums can be get using the algorithm in [2,3].

Consider the state transformation for the qubits after one CNOT operation with initial state \( \rho^{(0)} = |\psi^{(0)}\rangle \langle \psi^{(0)}| \). For the first step of CNOT gate, suppose the state for the qubits after this step is \( \rho^{(1)} \), the operator-sum representation of hyperoperator in quantum open system has the results \( \rho^{(1)} = \mathcal{E}(\rho^{(0)}) = \sum_i E_i \rho^{(0)} E_i^\dagger \). If we let
\[
M_1 = E_1 \otimes (E_1^\dagger)^T + E_2 \otimes (E_2^\dagger)^T + \cdots = E_1 \otimes E_1^* + E_2 \otimes E_2^* + \cdots,
\]
then \( \rho^{(1)} = M_1 \rho^{(0)} \). Here, \( \rho^{(0)} \) is straightening of matrix \( \rho \). Similarly, if we let the corresponding matrix of the second to fifth step be \( M_2, M_3, M_4, M_5 \), then
\[
\rho^{(1)} = M \rho^{(0)},
\]
here \( M = M_5 M_4 M_3 M_2 M_1 \).

According to the previous calculation, \( \rho^{(0)}, \rho^{(1)} \) are 12 × 12 matrices. Then \( \rho^{(0)} \), \( \rho^{(1)} \) are 144 × 1 column vectors. From Eq. (D.1), we can see that the matrix \( M \) corresponding to one CNOT operation is of the size 144 × 144. We need to determine the 144 × 144 elements. From Eq. (D.1), we can only get 144 equations. We have found other relation to get 144 × 144 equations, and finally get the matrix. Once \( M \) is obtained, from \( \rho^{(t)} = M_{t} \rho^{(0)} \), we can get the state after \( t \) times of CNOT operation \( \rho^{(t)} = M_{t} \rho^{(t-1)} = \cdots = M_{t} \rho^{(0)} \), then \( \rho^{(t)} \) is get.

\( \rho^{(t)} \) is a state with parameter \( \alpha_i (i = 1, \cdots, 12) \), then for different initial state, the actual \( \rho^{(t)} \) is different. We can get the failure probability of CNOT operations with the expected state and the actual state. The final results we reach is: the failure probability is of the order of \( 10^{-2} \) after \( 10^2 \) CNOT operations.

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Full quantum treatment of Rabi oscillation driven by pulse train and its application in ion-trap quantum computation

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Abstract. Rabi oscillations of two-level system driven by pulse train is a basic process involved in quantum computation. We give a full quantum treatment of this process, and show that the population inversion of this process collapses exponentially, has no revival phenomenon, and has a dual-pulse structure in every period. As an application, we investigate the properties of this process in ion-trap quantum computation. We find that in Cirac-Zoller computation scheme, when the wavelength of the driving field is of the order $10^{-6}$ m, the lower bound of failure probability is of the order $10^{-2}$ after about $10^2$ CNOT gates. This value is about the generally-accepted threshold in fault-tolerant quantum computation.

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1. Introduction

The presented quantum algorithms show that quantum computer (QC) can solve several famous problems intractable on classical computers [1], then challenge most public-key cryptosystems in use [2, 3]. Many proposals for implementing QC have been put forward. Among them, the cold ion trap scheme (Cirac-Zoller scheme) [4] is the earliest and most promising one, e.g., a scalable, multiplexed ion trap for quantum information processing has been demonstrated [5]. Implementation of quantum logic gates in this scheme is realized via Rabi oscillation of ions driven by pulse train of laser fields. The interaction of a single atom with radiation field is a basic interaction in physics. In [6], a nonperturbative fully quantum-theoretical analysis describing the transient spontaneous emission of an initially excited two-level atom in a one-dimensional cavity with output coupling is presented. In [7], they present observations of quantum dynamics of an isolated neutral atom stored in a magneto-optical trap.

The theoretic measure adapted in [4] is a typical one which takes the laser field as a classical field. However, considering the quantum nature of the driving field, one may get results which is different from the result under classical treatment. There are generally two ways to take account of the quantum nature of the field. One is to add quantum fluctuations to the classical treatment [8]. However, there are many operations in quantum computation, then in this case whether this method is suitable is still to be considered. The other way is to quantize the field and work out the result [9]. To do this, we first consider the Rabi oscillation driven by quantized pulse train. This is a basic atom-photon interaction process, and quantum computation is only one application of it. Then we can analyze the failure probability in ion-trap QC, and have further discussions.

Rabi oscillation driven by a quantized continuous-wave (cw) field, accompanied by collapse-revival phenomenon [10, 11, 12, 13], is a typical phenomenon of atom-photon systems. However, Rabi oscillation driven by quantized pulse train has not been fully investigated. Conceivably, it may have different phenomena compared with that driven by a cw field.

Fault-tolerant quantum computation (FTQC) allows the computer to work normally even when its elementary components are imperfect. However, the threshold theorem in FTQC requires the failure probability of each components below some threshold [14]. Then we can compare the failure probability with the value of threshold, and reach some meaningful conclusion in quantum computation [9].

This paper is arranged as follows: in Section 2 we describe a method to deal with quantum transformation of a two-level system after one coherent pulse, which expresses the relationship between the density matrices for the two-level system before and after one coherent pulse. In Section 3 we investigate the properties of Rabi oscillation driven by pulse train. In Section 4 we study this kind of Rabi oscillation in ion-trap quantum computation, and get the failure probability. In Section 5 we give out some discussions. In Section 6 some conclusions are reached.
2. Quantum transformation of a two-level system involving one coherent pulse

2.1. Modeling

The two-level system driven by repeated pulses is an open system, the usual way to deal with such a system is Kraus summation and master equation method. However, for the specific problem here, which cannot be easily solved with those methods, we study it in this way: after a single pulse, we get the density matrix for the whole system (including a two-level system and the laser field), then obtain the reduced density matrix for the two-level system. We can get the relation for the state of the two-level system before and after the pulse, then the state of the two-level system after repeated pulses can be get.

In [8, 15], they use the Jaynes-Cummings model (JCM) [16] for the case where an atom in the free space interacts with laser field. However, the JCM is the model to describe the interaction of atom and single-mode field in a cavity. Actually, there are some discussions [17, 18, 19] on the validation of the JCM in the multi-mode case. For example, in the paper by Enk and Kimble [15], at section 2.3 “Atom-light interaction”, they considered the case where an atom in free space interacts with a laser field, making use of Hamiltonian of JCM in Eq.(10). They also pointed out that the Hamiltonian in Eq. (10) in the paper is valid for atoms in free space for less than one Rabi period, but there is no strict proof.

We analyze the issue as follows: the sources of decoherence can generally lead to certain amount of failure probability on a single qubit or a pair of qubits. After many operations on the same qubit (or the same pair of qubits), the failure probability will generally accumulate to reach the threshold in the threshold theorem of FTQC. The corresponding operation number is the upper bound of operation number in one error-correction period when the given source of decoherence exists. Each source of decoherence considered can generally give corresponding upper bound of operation number, but this upper bound can be enlarged by technique improvement. When the upper bound increased to a huge value, it is actually not a bound.

The decoherence caused by field quantization can also give its upper bound of operation number. It is obtained theoretically, thus cannot be enlarged by technique improvement. The calculation of this decoherence should include the interaction of all modes in the radiation field with the two-level system. When using JCM, only one mode of the field is considered, and can also give an upper bound of operation number $\beta_1$. The accurate upper bound of operation number from field quantization $\beta < \beta_1$, because the spontaneous emission induced by vacuum modes is not considered in JCM. Then if we use JCM to estimate the upper bound of operation number in one error-correction period from field quantization, we can get meaningful results. The two-level system driven by pulse train can be described as

$$ H = \hbar g \left( e^{i\phi} \sigma_+ a + e^{-i\phi} a^\dagger \sigma_- \right), $$

(1)
Full quantum treatment of Rabi oscillation driven by pulse train

where \( g \) is the coupling constant, \( \phi \) is the beam phase, \( \sigma_+ \) and \( \sigma_- \) are the raising and lowering operators of the two-level system, and \( a^\dagger \) and \( a \) the creation and annihilation operators of photons, respectively. Then the unitary time-evolution operation is given by

\[
U(t) = \cos \left( g t \sqrt{a^\dagger a + 1} \right) |1\rangle\langle 1| + \cos \left( g t \sqrt{a^\dagger a} \right) |0\rangle\langle 0| - i \left[ e^{i\phi} \frac{\sin \left( g t \sqrt{a^\dagger a + 1} \right)}{\sqrt{a^\dagger a + 1}} a |1\rangle\langle 0| + e^{-i\phi} \frac{\sin \left( g t \sqrt{a^\dagger a + 1} \right)}{\sqrt{a^\dagger a + 1}} |0\rangle\langle 1| \right],
\]

with \(|0\rangle\) and \(|1\rangle\) the ground and excited state of the two-level system respectively.

Generally, the initial state of the whole system is \( |\psi(0)\rangle = \sum_{n=0}^{\infty} c_n |n\rangle \otimes (|\alpha\rangle + |\beta\rangle) \), where \( |c_n|^2 = \frac{\delta_{n,n}}{n!} \), and \( |\alpha|^2 + |\beta|^2 = 1 \). A single qubit gate is usually implemented through a \( k\pi \) pulse in Cirac-Zoller scheme, whose duration \( t_0 \) satisfies \( gt_0 \sqrt{n} = \frac{k\pi}{2} \) [15], with \( n \) the mean number of photons in the pulse. After a \( k\pi \) pulse, the state for the two-level system and laser field is

\[
|\psi_1\rangle = \alpha \left\{ \sum_{n=0}^{\infty} c_n \left[ \cos \left( \frac{k\pi \sqrt{n}}{2\sqrt{n}} \right) |0, n\rangle - i e^{i\phi} \sin \left( \frac{k\pi \sqrt{n}}{2\sqrt{n}} \right) |1, n-1\rangle \right] \right\} + \beta \left\{ \sum_{n=0}^{\infty} c_n \left[ \cos \left( \frac{k\pi \sqrt{n+1}}{2\sqrt{n}} \right) |1, n\rangle - i e^{-i\phi} \sin \left( \frac{k\pi \sqrt{n+1}}{2\sqrt{n}} \right) |0, n+1\rangle \right] \right\}.
\]

The corresponding density matrix for the state in (3) is \( \rho_{\text{total}}^{(1)} = |\psi_1\rangle\langle \psi_1| \). This matrix contains the information of both the two-level system and the field, but we are interested only in the two-level system. Thus we obtain the reduced density matrix

\[
\rho^{(1)} = \left[ |\alpha|^2 S_4 + \frac{1}{2} (|\alpha\beta^* - \alpha^*\beta| e^{i\phi} S_2 + |\beta|^2 (1 - S_4) + \alpha\beta^* S_5 + i(|\alpha|^2 e^{i\phi} S_1 - |\beta|^2 e^{-i\phi} S_7) + \alpha^*\beta S_3 \right],
\]

\[
S_1 = \sum_{n=0}^{\infty} \frac{e^{-\bar{n}n}}{n!} \sqrt{\frac{n}{n+1}} \cos \left( \frac{k\pi \sqrt{n}}{2\sqrt{n}} \right) \sin \left( \frac{k\pi \sqrt{n+1}}{2\sqrt{n}} \right),
\]

\[
S_2 = \sum_{n=0}^{\infty} \frac{e^{-\bar{n}n}}{n!} \sqrt{\frac{k\bar{n}}{2(n+1)}} \sin \left( \frac{k\pi \sqrt{n+1}}{\sqrt{n}} \right),
\]

\[
S_3 = \sum_{n=0}^{\infty} \frac{e^{-\bar{n}n}}{n!} \sqrt{\frac{n}{n+1}} \sin \left( \frac{k\pi \sqrt{n+1}}{2\sqrt{n}} \right) \sin \left( \frac{k\pi \sqrt{n+1}}{2\sqrt{n}} \right),
\]

\[
S_4 = \sum_{n=0}^{\infty} \frac{e^{-\bar{n}n}}{n!} \cos^2 \left( \frac{k\pi \sqrt{n}}{2\sqrt{n}} \right),
\]

\[
S_5 = \sum_{n=0}^{\infty} \frac{e^{-\bar{n}n}}{n!} \cos \left( \frac{k\pi \sqrt{n}}{2\sqrt{n}} \right) \cos \left( \frac{k\pi \sqrt{n+1}}{2\sqrt{n}} \right),
\]

\[
S_6 = \sum_{n=0}^{\infty} \frac{e^{-\bar{n}n}}{n!} \cos^2 \left( \frac{k\pi \sqrt{n+1}}{2\sqrt{n}} \right),
\]

(4)
2.2. Transforms of the density matrix after a coherent pulse

Consider the relationship between \( \rho^{(1)} \) and the density matrix of corresponding initial state \( \rho^{(0)} = |\psi(0)\rangle \langle \psi(0)| \). For a two-level system, the density matrix \( \rho \) satisfies the condition \( \rho = \frac{1}{2}(I + r \cdot \sigma) \) \( [14] \), \( r \) is the Bloch vector for state \( \rho \), \( |r| \leq 1 \), \( \sigma = \begin{bmatrix} \sigma_x & \sigma_y & \sigma_z \end{bmatrix}^T \).

Let \( r^{(m)} = \begin{bmatrix} r_x^{(m)} & r_y^{(m)} & r_z^{(m)} \end{bmatrix}^T \) denotes the Bloch vector of \( \rho^{(m)} \). An arbitrary trace-preserving quantum operation is equivalent to a map of the form \( r \xrightarrow{E} r’ = Mr + c \) \( [14] \), here \( M \) and \( c \) contain the properties of the system and are independent of the state. Based on this, it can be seen that \( r^{(1)} = Mr^{(0)} + c \), here \( c = \begin{bmatrix} 0 & S_7 e^{-i\phi} - S_1 e^{i\phi} & S_4 + S_6 - 1 \end{bmatrix}^T \),

\[
M = \begin{bmatrix} S_3 + S_5 & 0 & 0 \\ 0 & M_1 & 0 \\ 0 & 0 & M_2 \end{bmatrix}, \quad M_1 = \begin{bmatrix} S_5 - S_3 & -(e^{i\phi}S_1 + e^{-i\phi}S_7) \\ S_2 e^{i\phi} & S_4 - S_6 \end{bmatrix},
\]

then \( r^{(m)} = Mr^{(m-1)} + c \).

2.3. Calculation of the sums in the density matrix

It is necessary to get accurate values of \( S_i \) \( (i = 1, \cdots, 7) \) to evaluate the behavior of pulse train. The usual algorithm (saddle-point approximation) can only reach a precision of \( 1/\sqrt{n} \). Our algorithm achieving any given precision instead of the usual algorithm is as follows.

Suppose \( \bar{n} \) is not small, for the sum

\[
\sum_{n=0}^{\infty} \frac{e^{-n\bar{n}}}{n!} f_{i0}(n, \bar{n}, k),
\]

(1) Substitute \( n \) in \( f_{i0}(n, \bar{n}, k) \) with \( (x+1)\bar{n} \), we get \( f_{i1}(x, \bar{n}, k) = f_{i0}((x+1)\bar{n}, \bar{n}, k) \).

(2) Do Taylor expansion to \( x^p \) for \( f_{i1}(x, \bar{n}, k) \) at \( x = 0 \), and get \( f_{i2}(x, \bar{n}, k) \).

(3) Since sum \( \sum_{n=0}^{\infty} \frac{e^{-n\bar{n}}}{n!} n^k \) can be get accurately, we replace \( x \) in \( f_{i2}(x, \bar{n}, k) \) by \( x^k \) and get \( f_{i3}(n, \bar{n}, k) \).

(4) Use \( f_{i3}(n, \bar{n}, k) \) instead of \( f_{i0}(n, \bar{n}, k) \) in the expression of \( S_i(\bar{n}, k) \) to calculate the new sum and get \( f_{i4}(\bar{n}, k) \).

(5) Substituting \( \bar{n} \) into \( f_{i4}(\bar{n}, k) \), we obtain a high-precision result of the original sum \( S_i(\bar{n}, k) \). The value for \( S_i \) \( (i = 1, \cdots, 7) \) in the cases where we expand \( f_{i1}(x, \bar{n}, k) \) to \( x^{10} \) and \( x^{15} \) are compared in Table I.

The precision of the sums \( S_i(i = 1, 2, \cdots, 7) \) is ensured by the following theorem:
Table 1: Values for $S_i(i = 1, 2, \cdots, 7)$ for $\bar{n} = 10^4$ and $k = 2$. “Value1” denotes value of the resulting sums of the algorithm when we expand $f_{i1}(x, \bar{n}, k)$ to $x^{10}$ and “Value2” denotes that when we expand $f_{i1}(x, \bar{n}, k)$ to $x^{15}$. Value1 and Value2 are the same to the precision $10^{-23}$.

| Sum  | Value1             | Value2             |
|------|--------------------|--------------------|
| $S_1$ | 0.000 039 303 916 656 063 668 561 519 091 | 0.000 039 303 916 656 063 668 561 194 770 |
| $S_2$ | 0.000 039 265 164 255 300 772 996 074 590 | 0.000 039 265 164 255 300 772 995 750 283 |
| $S_3$ | 0.000 246 659 192 761 352 167 541 307 293 | 0.000 246 659 192 761 352 167 542 042 758 |
| $S_4$ | 0.999 753 309 972 685 637 856 777 333 369 | 0.999 753 309 972 685 637 856 776 237 858 |
| $S_5$ | 0.999 753 316 133 881 571 308 212 070 145 | 0.999 753 316 133 881 571 308 210 974 684 |
| $S_6$ | 0.999 753 322 301 165 250 291 025 614 276 | 0.999 753 322 301 165 250 291 024 518 866 |
| $S_7$ | 0.000 039 226 416 698 193 975 826 600 887 | 0.000 039 226 416 698 193 975 830 095 264 |

**Theorem 1:** For every given integer $l << \bar{n}$, let

$$p = \frac{\ln \left( \sqrt{2\bar{n}^{l+\frac{1}{2}}(l+1)\ln \bar{n}} \right)}{\frac{1}{2} \ln \bar{n} - \ln \left( (l+1)\ln \bar{n} \right)}$$  \hspace{1cm} (5)

$$\alpha_0 = \frac{1}{\sqrt{\bar{n}}} + \frac{(l+1)\ln \bar{n}}{\sqrt{\bar{n}}} + \sqrt{\frac{(l+1)^2(\ln \bar{n})^2}{\bar{n}}} + 2(l+1)\ln \bar{n}.$$  \hspace{1cm} (6)

If $\alpha_0 < \alpha << \sqrt{\bar{n}}$, then

$$\sum_{n=0}^{\infty} \frac{e^{-\bar{n}\bar{n}^n}}{n!} f_{i0}(n, \bar{n}, k) = \sum_{n=0}^{\infty} \frac{e^{-\bar{n}\bar{n}^n}}{n!} f_{i3}(n, \bar{n}, k) + o\left(\frac{1}{\bar{n}^l}\right),$$  \hspace{1cm} (7)

here $p, f_{i0}(n, \bar{n}, k), f_{i3}(n, \bar{n}, k)$ are parameters defined in the algorithm above.

Theorem 1 can be proved using the following three lemmas (see Appendix A for the detailed proof):

**Lemma 1:** For every given $\alpha << \sqrt{\bar{n}}$,

$$\sum_{n=\bar{n} - \alpha\sqrt{\bar{n}}}^{\bar{n} + \alpha\sqrt{\bar{n}}} \frac{e^{-\bar{n}\bar{n}^n}}{n!} \left( f_{i0}(n, \bar{n}, k) - f_{i3}(n, \bar{n}, k) \right) = o\left( \frac{\alpha^{p+1}}{(\sqrt{\bar{n}})^{p-1}} \right).$$  \hspace{1cm} (7)

here $p, f_{i0}(n, \bar{n}, k), f_{i3}(n, \bar{n}, k)$ are parameters defined in the algorithm above.

**Lemma 2:** For every given integer $l << \bar{n}$, $\alpha << \sqrt{\bar{n}}$, if $\alpha > \sqrt{(l+1)\ln \bar{n}}$, then

$$\sum_{n=0}^{k} \frac{e^{-\bar{n}\bar{n}^n}}{n!} < \frac{1}{\bar{n}^l},$$  \hspace{1cm} (8)

where $k = \lceil \bar{n} + \alpha\sqrt{\bar{n}} \rceil$.

**Lemma 3:** For every given integer $l << \bar{n}$, $\alpha << \sqrt{\bar{n}}$, if

$$\alpha > \frac{1}{\sqrt{\bar{n}}} + \frac{(l+1)\ln \bar{n}}{\sqrt{\bar{n}}} + \sqrt{\frac{(l+1)^2(\ln \bar{n})^2}{\bar{n}}} + 2(l+1)\ln \bar{n},$$  \hspace{1cm} (9)

then

$$\sum_{n=k}^{\infty} \frac{e^{-\bar{n}\bar{n}^n}}{n!} < \frac{1}{\bar{n}^l}.$$
  \hspace{1cm} (10)
where \( k' = \lceil \bar{n} + \alpha \sqrt{n} \rceil \).

We expand \( f_1(x, \bar{n}, k) \) to \( x^{15} \) at \( x = 0 \), and find the value of the sum is the same to the precision \( 10^{-23} \) as that when we expand \( f_1(x, \bar{n}, k) \) to \( x^{10} \). It implies that the precision of the sum is much higher than Eq. (5) shows. The reason is probably that we have not considered the periodicity of trigonometric functions, and the precision of the sum may be remarkably improved since the positive and negative terms will cancel each other out.

For small \( \bar{n} \), we need only to require \( t \) satisfying
\[
(t - 1)! > e^{-\bar{n}t^2},
\]
where \( t \) is the parameter in sum \( S_i(\bar{n}, k) = \sum_{n=0}^{t} \frac{e^{-\bar{n}n^2}}{n!} f_{i0}(n, \bar{n}, k) + o \left( \frac{1}{m^2} \right) \). For a given precision \( l \), we can search out the smallest \( t \) satisfying (11), e.g., when \( \bar{n} = 10 \) and \( l = 20 \), we get \( t = 55 \).

3. Population inversion

3.1. Final state of the two-level system after pulse train

Provided \( r^{(m)} = Mr^{(m-1)} + c \), then
\[
r^{(m)} = M^m r^{(0)} + (M^{m-1} + \cdots + M + I)c.
\]

It can be seen from Sec. 2.2 that
\[
M^m = \begin{bmatrix} (S_3 + S_5)^m & 0 \\ 0 & M_1^m \end{bmatrix},
M_1 = \begin{bmatrix} S_5 - S_3 & -(S_1 + S_7) \\ S_2 & S_4 + S_6 - 1 \end{bmatrix},
\]
where \( \Lambda_1 = \lambda_1^m + \lambda_2^m \) with \( \lambda_1 \) and \( \lambda_2 \) eigenvalues of \( A \), \( K = d - a, Q = -i\sqrt{(a - d)^2 + 4bc} \). When \((a - d)^2 + 4bc < 0\) (which is the case for \( M_1 \))
\[
A^m = \frac{\Lambda_+^m}{2} I + \frac{\Lambda_-^m}{2iQ} \begin{bmatrix} -K & 2b \\ 2c & K \end{bmatrix},
\]
where \( \Lambda_{\pm}^m = \lambda_1^m \pm \lambda_2^m \) with \( \lambda_1 \) and \( \lambda_2 \) eigenvalues of \( A \), \( K = d - a, Q = -i\sqrt{(a - d)^2 + 4bc} \). When \((a - d)^2 + 4bc < 0\) (which is the case for \( M_1 \))
\[
A^m = |\lambda|^m \begin{bmatrix} \cos(m\theta) I + \sin(m\theta) J \sqrt{\det J} \end{bmatrix},
\]
where \( |\lambda|^2 = ad - bc \), \( \sin \theta = \frac{1}{2} \sqrt{2 - \frac{a^2 + d^2 + 2bc}{ad-bc}} \), \( J = \begin{bmatrix} a - d & 2b \\ 2c & d - a \end{bmatrix} \). Therefore,
\[
I + M_1 + \cdots + M_1^{m-1} = \left[ \sum_{j=0}^{m-1} |\lambda|^j \cos(j\theta) \right] I + \left[ \sum_{j=0}^{m-1} |\lambda|^j \sin(j\theta) \right] \frac{J}{\sqrt{\det J}}.
\]
Since
\[
\sum_{j=0}^{m-1} \{|\lambda|^j \cos(j\theta) + i \sin(j\theta)|\} = \sum_{j=0}^{m-1} (|\lambda|^j e^{i(j\theta)}) = \sum_{j=0}^{m-1} (|\lambda| e^{i\theta})^j
\]
\[
= \frac{1 - |\lambda| e^{-i\theta} - |\lambda|^m e^{i(m\theta)} + |\lambda|^{m+1} e^{i(m-1)\theta}}{1 + |\lambda|^2 - 2|\lambda| \cos \theta},
\]
we have
\[
\sum_{j=0}^{m-1} |\lambda|^j \cos(j\theta) = \frac{1 - |\lambda| \cos \theta - |\lambda|^m \cos(m\theta) + |\lambda|^{m+1} \cos(m-1)\theta}{1 + |\lambda|^2 - 2|\lambda| \cos \theta},
\]
\[
\sum_{j=0}^{m-1} |\lambda|^j \sin(j\theta) = \frac{|\lambda| \sin \theta - |\lambda|^m \sin(m\theta) + |\lambda|^{m+1} \sin(m-1)\theta}{1 + |\lambda|^2 - 2|\lambda| \cos \theta},
\]
thus
\[
I + M_1 + \cdots + M_1^{m-1}
\]
\[
= \frac{1}{1 + |\lambda|^2 - 2|\lambda| \cos \theta} \left[ (1 - |\lambda| \cos \theta - |\lambda|^m \cos(m\theta) + |\lambda|^{m+1} \cos(m-1)\theta) I + \right.
\]
\[
\left. \frac{|\lambda| \sin \theta - |\lambda|^m \sin(m\theta) + |\lambda|^{m+1} \sin(m-1)\theta}{1 + |\lambda|^2 - 2|\lambda| \cos \theta} \frac{J}{\sqrt{\det J}} \right] \Delta B_1^{(m)} I + B_2^{(m)} J,
\]
then
\[
r^{(m)} = \begin{bmatrix}
(S_3 + S_5)^m & 0 \\
0 & |\lambda|^m \end{bmatrix} \begin{bmatrix}
0 \\
\frac{1}{\sqrt{\det J}} \cos(m\theta) I + \sin(m\theta) \frac{J}{\sqrt{\det J}}
\end{bmatrix}
\]
\[
+ \begin{bmatrix}
1-(S_3+S_5)^m \\
0 \\
O \\
0 \\
1-S_3-S_5
\end{bmatrix}
\begin{bmatrix}
B_1^{(m)} I + B_2^{(m)} J
\end{bmatrix} c.
\]

3.2. Population inversion after pulse train

Suppose the initial state is $|1\rangle$, if we have applied $k\pi$ pulses for $m$ times, the population inversion is
\[
W_m = \frac{1}{2} (1 - r_z^{(m)}) - \frac{1}{2} (1 + r_z^{(m)}) = -r_z^{(m)},
\]
we have
\[
W_m = |\lambda|^m \left[ \cos(m\theta) + \sin(m\theta) \frac{\dot{j}_{22}}{\sqrt{\det J}} \right] - \frac{1}{1 + |\lambda|^2 - 2|\lambda| \cos \theta}
\]
\[
\times \left\{ \left[ |\lambda| \sin \theta - |\lambda|^m \sin(m\theta) + |\lambda|^{m+1} \sin(m-1)\theta \right] \frac{\dot{j}_{21}}{\sqrt{\det J}} (S_7 - S_1) 
\right.
\]
\[
+ \left[ \left( 1 - |\lambda| \cos \theta - |\lambda|^m \cos(m\theta) + |\lambda|^{m+1} \cos(m-1)\theta \right) 
\right.
\]
\[
+ \left( |\lambda| \sin \theta - |\lambda|^m \sin(m\theta) + |\lambda|^{m+1} \sin(m-1)\theta \right) \frac{\dot{j}_{22}}{\sqrt{\det J}} (S_4 - S_6) \right\}. \tag{14}
\]
Full quantum treatment of Rabi oscillation driven by pulse train

To get the inversion between the $m$th and $(m+1)$th $k\pi$ pulse, we should first get the corresponding density matrix of the two-level system
\[
\rho_m(t) = \text{tr}\left\{U(t)[\rho^{(m)} \otimes \rho_1]U^\dagger(t)\right\},
\]
where $U(t)$ is the unitary time-evolution operator mentioned earlier, and $\rho_1$ is the density matrix for the laser field. A detailed calculation gives the probability that the ion is in state $|0\rangle$:
\[
p(t) = \frac{1}{2}\left[(S_8 + S_9) + r_x^{(m)}(t)(S_8 - S_9) + r_y^{(m)}(t)S_{10}\right],
\]
where $S_8 = \sum_{n=0}^{\infty} \frac{e^{-n\bar{n}}}{n!} \cos^2 gt\sqrt{n}$, $S_9 = \sum_{n=0}^{\infty} \frac{e^{-n\bar{n}}}{n!} \sin^2 gt\sqrt{n+1}$ and $S_{10} = \sum_{n=0}^{\infty} \frac{e^{-n\bar{n}}}{n!} \sqrt{\frac{\pi}{n}} \sin 2gt\sqrt{n}$, which can all be got with high precision using our algorithm in Section 2.3, and the inversion is $W_m(t) = 1 - 2p(t), 0 < t < \frac{k\pi}{2\sqrt{2}V}$.

Now think of the difference of the oscillation driven by pulse train and a cw field. The population inversion for repeated $2\pi$ pulses is shown in Figure 1a (given $\bar{n} = 10$). We find there is a dual-pulse structure in every period, where the amplitude starts to increase from the point of $2\pi$ pulses. The inversion decreases exponentially, different from a Gaussian function collapse envelope driven by a cw field. Besides, there is no revival phenomenon, but a small nonzero amplitude exists. The reason for this behavior is probably that the system we consider here is an open quantum system with dissipation.

The inversion at the points of $2\pi$ pulses when $\bar{n} = 10^4$ is plotted in Figure 2. Results of fitting is $1.0031e^{-0.0002N_R}$, $1.0193e^{-0.0003N_R}$, $1.025e^{-0.0005N_R}$ for $k = 1/2, 1, 2$ respectively, here $N_R$ is the number of Rabi periods.

4. Failure probability of gate operation realized through Rabi oscillation driven by repeated pulses

4.1. Estimation of $\bar{n}$

$\bar{n}$ which determines $S_8$ is an important parameter in our discussion. To estimate the mean number of photons in one pulse, we assume a fictitious pulse propagating in the opposite direction at the same time. They form a standing wave instantly while overlapping in space. It can be seen that the mean number of photons in each pulse is about half of that in the standing wave. We now focus on mean number of photons in the imagined standing wave.

The electric field $E$ can be expressed as $E = E\sqrt{\bar{n}}$. $E$ is usually given as $E = \sqrt{\frac{\omega_0}{e a_0}}$ [20], where $\omega$ is the frequency of the single mode in a cavity, and $V$ is the volume of the cavity. It can be seen that $V \sim Act$, with $A$ the cross-sectional area of the beam, thus $\bar{n} = \frac{\omega_0 Act}{h}E^2$. For a $k\pi$ pulse, $gt\sqrt{\bar{n}} = \frac{k\pi}{2}$, $g \sim \frac{\omega E}{\hbar V\sqrt{\bar{n}}}$, with $p \sim ea_0$ the electric dipole moment of the ion, $e$ the charge of an electron, and $a_0$ Bohr radius, then we get $t = \frac{k\pi\hbar}{2pE}$. Then we have $\bar{n} = \frac{k\pi a_0\hbar}{2pE}$.

When the laser beam interacts with an ion, not all the photon in the beam are effective. Think of the effective mean number of photons. When a laser beam is
Figure 1: Population inversion driven by different fields, given $\bar{n} = 10$, $\tau = g t$. (a) $2\pi$ pulse train case. There is a dual-pulse structure in every period, where the amplitude starts to increase from the point of $2\pi$ pulses. The inversion decreases exponentially, different from a Gaussian function collapse envelope driven by a cw field. Besides, there is no revival phenomenon, but a small nonzero amplitude exists. (b) Corresponding inversion driven by a cw field.

applied to a trapped ion, the total resonant scattering cross section for an atomic dipole transition is $\sigma = 3\lambda^2/2\pi$ [21], and the cross section for scattering out of the paraxial modes is $\sigma_{\text{eff}} = 3\lambda^2/8\pi$ [22]. Then the effective interaction area is $\sigma_{\text{eff}}$, and the photons in volume $\sigma_{\text{eff}} c t$ is effective. For each photon, the probability to be in area $\sigma_{\text{eff}}$ is $\frac{\sigma_{\text{eff}}}{A}$, and the probability are independent for the photons. It can be seen that the effective
Full quantum treatment of Rabi oscillation driven by pulse train

Figure 2: Inversion at the points of $2\pi$ pulses $E(W)$ versus number of Rabi periods $N_R$, $\bar{n} = 10^4$. Fitting results are $1.0031e^{-0.0002N_R}$, $1.0193e^{-0.0003N_R}$, $1.025e^{-0.0005N_R}$ for $k = 1/2, 1, 2$ respectively.

Mean number of photons is

$$\bar{n}_{eff} = \frac{n_{eff}}{A} = \frac{k}{4} \frac{e_0 \sigma_{eff} \lambda}{p} E.$$  \hfill (16)

One case people are interested in is the sideband transition, where the laser detuning $\Delta = \pm \omega_t$, here $\omega_t$ is the frequency of the trap. Because of AC-Stark shift and off-resonant transitions, the sideband Rabi frequency $\Omega_+$ has upper bound \[23\]. People have adopted methods to partially cancel the effect, and it seems feasible to have $\Omega_+ < \omega_t$ for special temporal and spectral arrangements of the laser field \[24\]. Since $\Omega_+ = \frac{2\pi}{\lambda} \sqrt{\frac{h}{2M \omega_t}} \Omega$, with $M$ the mass for a single ion, we have

$$\Omega < \frac{\lambda}{2\pi} \sqrt{\frac{2M}{\hbar}} \omega_t^{\frac{3}{4}}.$$  \hfill (17)

From \[25\] and \[26\], it can be seen that

$$\Omega = -\frac{e a_0 E}{4h} = \frac{p E}{4h},$$

$$\omega_t = \sqrt{\frac{e^2}{4\pi \epsilon_0 M z_s^3}},$$  \hfill (18)

where $z_s$ is the order of the separation between ions and is typically 10 to 100 $\mu$m. Suppose $z_s = \xi \lambda$, from (17) and (18), we get

$$E < \frac{2\sqrt{2\hbar}}{p\pi} \left( \frac{e^2}{4\pi \epsilon_0} \right)^{\frac{3}{4}} M^{-\frac{1}{4}} \xi^{-\frac{1}{2}} \lambda^{-\frac{3}{4}}.$$  \hfill (19)

Substitute back to (16), we get

$$\bar{n} < \frac{3e_0^4}{32a_0^2 p\pi^{\frac{11}{4}}} \sqrt{\frac{\hbar}{e}} kM^{-\frac{1}{4}} \xi^{-\frac{9}{4}} \lambda^{\frac{7}{4}}$$

$$= 6 \times 10^7 kM^{-\frac{1}{4}} \xi^{-\frac{9}{4}} \lambda^{\frac{7}{4}}.$$  \hfill (20)
In the cases we consider, it is suitable to limit \(k \leq 2\), \(9u \leq M \leq 200u\) (\(u = 1.66057 \times 10^{-27}\) kg). For \(M = 9u\), \(k = 2\), we get

\[
\bar{n} = 3.4 \times 10^{14} \xi^{-\frac{2}{7}} \lambda^{\frac{7}{4}}.
\]

We can see that a large \(\lambda\) and a small \(\xi\) result in a large \(\bar{n}\). The curves of \(\lg(\bar{n})\) is plotted in Figure 3 versus parameter \(\xi\) from 2 to 100. When \(\lambda = 10^{-6}\) m and \(\xi = 2\), we get \(\bar{n} = 2.3 \times 10^3\).

![Figure 3: Logarithm of mean number of photons \(\lg(\bar{n})\) as a function of \(\xi\) and \(\lambda\). It can be seen that \(\bar{n}\) increases with \(\lambda\) and decreases with \(\xi\).](image)

There are also authors calculating \(\bar{n}\) in a \(k\pi\) pulse in another way \[15\]: they considered the situation where a single laser is used to drive Rabi oscillation of the atom, and adopted the formalism introduced by Blow et al. \[27\], taking the laser as a continuous-mode coherent state. They worked out the interaction time \(t\) for \(k\pi\) pulse as \(t = \frac{k\pi h}{d} \sqrt{\frac{\alpha c A}{2P}}\), where \(d\) is the coupling constant of the atom and laser, and \(P\) is the power of the laser. Thus, the mean number of photons in one \(k\pi\) pulse is \(\bar{n} \approx \frac{P t}{\hbar \omega_L} = \frac{k\pi}{\omega_L d} \sqrt{\frac{\alpha c A P}{2}}\), where \(\omega_L\) is the frequency of the representative single-mode coherent state. Thus, obviously, they take all the photons in area \(A\) as effective photons when considering the interaction, but actually the number of effective photons is much smaller.

4.2. Accuracy of gate operation

Suppose we have applied \(m\) times of coherent pulses and reached a state \(\rho^{(m)} = \frac{1}{2}(I + r^{(m)} \cdot \sigma)\). Let \(|\Psi\rangle = \alpha|0\rangle + \beta|1\rangle\) be the expected state, the accuracy rate of gate operation realized through Rabi oscillation is

\[
p_s^{(m)} = (\alpha^*|0\rangle + \beta^*|1\rangle)\rho^{(m)}(\alpha|0\rangle + \beta|1\rangle) = |

\[
= |\alpha|^2 \rho^{(m)}_{11} + |\beta|^2 \rho^{(m)}_{22} + \alpha^* \beta \rho^{(m)}_{12} + \alpha \beta^* \rho^{(m)}_{21}

\[
= \frac{1}{2} \left(1 + r_z^{(m)} r_z^{(m)} + r_x^{(m)} r_x^{(m)} + r_y^{(m)} r_y^{(m)}\right)

\[
= \frac{1}{2} (1 + r^{(0)} \cdot r^{(m)}),
\]
for a mixed state, $|r^{(m)}| < 1$, then $p_s < 1$. The failure probability is $p_f^{(m)} = 1 - p_s^{(m)}$. A detailed calculation results (see Appendix C)

$$p_f^{(m)} = -\frac{1}{2}(r^{(0)} \cdot r^{(m)} - 1)$$

$$= -\frac{1}{2}\left\{ (r_x^{(0)})^2[(S_3 + S_5)^m - 1] + ((r_y^{(0)})^2 + (r_z^{(0)})^2)[|\lambda|^m \cos(m\theta) - 1] + |\lambda|^m \sin(m\theta)(\det J)^{-\frac{1}{2}}[((r_y^{(0)})^2 - (r_z^{(0)})^2)(a - d) + r_y^{(0)}r_z^{(0)}(b + c)] + B_1^{(m)}(r_y^{(0)}c_y + r_z^{(0)}c_z) + B_2^{(m)}[(r_y^{(0)}c_y - r_z^{(0)}c_z)(a - d) + r_y^{(0)}c_y c + r_z^{(0)}c_z b]\right\}.$$

Then we average over all initial states of the ion, and get the average failure probability. The failure probability for $k\pi$ pulses with different $\bar{n}$ are shown in Figure 4. It can be seen that the failure probability increases with the number of Rabi periods $N_R$ and the value $k$, and is inversely proportional to $\bar{n}$.

![Figure 4](image_url)

**Figure 4:** Failure probability $p_f$ versus number of Rabi periods $N_R$, $k\pi$ pulses are applied, and $\bar{n}$ is $10^4$ ($10^6$) in (a) (b). The failure probability $p_f$ increases with the number of Rabi periods $N_R$ and the value $k$, and is inversely proportional to $\bar{n}$.

5. Discussions

5.1. The reason for tracing out the laser field after each pulse

For the Cirac-Zoller CNOT scheme, there are five steps to implement it. The laser phase in the five steps are $\pi/2$, 0, 0, 0 and $-\pi/2$, which are correlated. However, there is no correlation between two different CNOT gates. Then after completing one CNOT gate, it is valid to trace out the laser field. The calculation in Sec. 2 for different pulses is an analog of different CNOT gates. This treatment is meaningful for our purpose, i.e., to estimate the lower bound of failure probability, or the upper bound of operation.
number, after many CNOT operations. More-detailed analysis of the lower bound of failure probability after Cirac-Zoller CNOT operations can be seen in [28], which is to be published.

5.2. The permitted depth of quantum logical operation

Failure probability we have calculated for the $\pi$ sideband transition amounts to $10^{-2}$ after approximately $10^2$ operations when $\bar{n} = 10^4$. For controlled-NOT (CNOT) gates, there are five steps in Cirac-Zoller scheme, and two steps are realized via Rabi oscillations driven by $\pi$ pulses. Generally speaking, the failure probability after five steps is not less than that after one $\pi$ pulse. Then the failure probability after repeated $\pi$ pulses is a lower bound of the failure probability after repeated Cirac-Zoller’s CNOT gate. Thus the lower bound of the failure probability is $10^{-2}$ after approximately $10^2$ CNOT operations when $\bar{n} = 10^4$.

The threshold theorem in quantum computation declares that an arbitrarily long quantum computation can be performed reliably if the failure probability of each quantum gate is less than a critical value. Knill used numerical calculations and obtained a threshold of the order $10^{-2}$ [29] based on a fault-tolerant structure suggested by himself. P. Aliferis et al. reached a threshold of $10^{-3}$ with provable constructions [30].

A parameter called permitted depth of logical operation describing the property of a physical realization scheme of QC has been given [9]: considering that different number state components of the driving field lead to different oscillation amplitudes, which become uncorrelated gradually, we can see that failure probability of quantum logic gates has a theoretical limitation. Combing this limitation given by the quantum nature of the field with the threshold theorem in FTQC, we can get permitted depth of logical operation. This parameter limits the number of operations on any physical qubit in one error-correction period. Then the permitted depth of logical operation here is less than $10^2$.

5.3. Others’ proposals which may have different results

For Rabi oscillation driven by microwaves, the failure probability may be much smaller because of a large mean number of photons, but it becomes difficult to individually address each ions. Although an additional magnetic field gradient applied to an electrodynamic trap may individually shift ionic qubit resonances [31], thus making them distinguishable in frequency space, whether it can improve the permitted depth of logical operation needs further investigation.

There exists a two-qubit gate scheme totally different from the Cirac-Zoller gate, such as the scheme implemented by the NIST group [32]. In the scheme off-resonant excitations of the stronger carrier transition is absent, and this allows a greater gate speed thus a higher laser intensity. Besides, additional Stark shifts can be efficiently suppressed by choosing almost perpendicular and linear polarizations for the laser beams [33]. Hence, studies on this type of gate may lead to different results.
6. Conclusions

Firstly, we investigate Rabi oscillation of a two-level system driven by pulse train. We develop an algorithm to solve the infinite summation, with a high precision which has never been reached by former authors. We find that in this kind of Rabi oscillation, there is a dual-pulse structure in every period. The envelope of population inversion collapses exponentially, different from a Gaussian function collapse envelope driven by a cw field. Besides, there is no revival phenomenon, but an approaching to a tiny platform.

Secondly, we consider the application to gate operation in ion trap quantum computation. We give a lower bound of failure probability. Our result is: that when the wavelength of the driving field is of the order $10^{-6}$ m, the mean number of photons cannot be greater than $10^4$. Then, after about $10^2$ CNOT gates in Cirac-Zoller scheme, the lower bound of failure probability is of the order $10^{-2}$.

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Appendix A. PROOF OF PRECISION OF THE ALGORITHM IN SEC.

Proof of Lemma 1: For $\bar{n} - \alpha \sqrt{n} < n < \bar{n} + \alpha \sqrt{n}$, i.e. $-\frac{\alpha}{\sqrt{n}} < x < \frac{\alpha}{\sqrt{n}}$, after expanding $f_{i1}(x, \bar{n}, k)$ at $x = 0$, we get the result $f_{i2}(x, \bar{n}, k) = f_{i0}(n, \bar{n}, k) + o(x^p)$. It can be seen that $f_{i2}(x, \bar{n}, k) = f_{i3}(n, \bar{n}, k)$, thus we have $f_{i0}(n, \bar{n}, k) = f_{3}(n, \bar{n}, k) + o(x^p)$, then Eq. (7) is proved □

Proof of Lemma 2: For every given $n$ satisfying $n < k + 1 < \bar{n}$, we have $\frac{\bar{n}^j}{n!} < \frac{\bar{n}^{k+1}}{(k+1)!}$, thus

$$\sum_{n=0}^{k} e^{-\bar{n}} \frac{\bar{n}^j}{n!} < \sum_{n=0}^{k} e^{-\bar{n}} \frac{\bar{n}^{k+1}}{(k+1)!} = e^{-\bar{n}} \frac{\bar{n}^{k+1}}{k!}.$$  \hspace{1cm} (A.1)

From Stirling's formula $k! = \sqrt{2\pi k} \left(\frac{k}{e}\right)^k e^{\frac{\theta}{12}}$, $0 < \theta < 1$, we have

$$e^{-\bar{n}} \frac{\bar{n}^{k+1}}{k!} < \left(\frac{e}{k}\right)^k e^{-\bar{n}} \bar{n}^{k+1} = e^{k-\bar{n}} \bar{n} \left(\frac{k}{\bar{n}}\right)^{k+1}.$$  \hspace{1cm} (A.2)

Substitute $k$ in formula (A.2) with $\bar{n} - \alpha \sqrt{n}$, we have

$$e^{k-\bar{n}} \bar{n} \left(\frac{k}{\bar{n}}\right)^{k+1} = \bar{n} e^{-\alpha \sqrt{n}} (1 - \frac{\alpha}{\sqrt{n}})^{\frac{\alpha}{\sqrt{n}} (\alpha \sqrt{n} - \alpha^2)}$$

$$= \bar{n} e^{-\alpha \sqrt{n}} e^{a \sqrt{n} - \alpha^2} = \bar{n} e^{-\alpha^2}.$$  \hspace{1cm} (A.3)

When $\alpha > \sqrt{(l+1) \ln \bar{n}}$, we have $\bar{n} e^{-\alpha^2} < \frac{1}{\bar{n}^l}$, inequality (8) is proved. □
Proof of Lemma 3: It can be seen that
\[
\sum_{n=k'}^{\infty} \frac{e^{-\bar{n}} \bar{n}^n}{n!} = e^{-\bar{n}} \sum_{n=k'}^{\infty} \frac{\bar{n}^{n-k'} k'^!}{n!} < e^{-\bar{n}} \frac{\bar{n}^{k'+1}}{k'^!} \sum_{n=k'}^{\infty} (\frac{\bar{n}}{k'^!})^{n-k'} = e^{-\bar{n}} \frac{\bar{n}^{k'+1}}{k'^!} k'^! + \frac{1}{k'^!}.
\]
when \(k' > \bar{n} + \frac{1}{\eta},\) i.e., \(\frac{k'+1}{\bar{n}+1-\bar{n}} < k',\) we have
\[
e^{-\bar{n}} \bar{n}^{k'+1} < (\frac{e}{k'})^{k'} e^{-\bar{n}} \bar{n}^{k'+1} < \bar{n} e^{-\bar{n}} \bar{n}^{k'-1} (k' - 1)!.
\]
with Stirling’s formula we get
\[
\left(\frac{e}{k'}\right)^{k'} e^{-\bar{n}} \bar{n}^{k'+1} < \bar{n} e^{-\bar{n}} \bar{n}^{k'-1} (k' - 1)! < \bar{n} e^{-\bar{n}} \bar{n}^{k'-1} = \bar{n} e^{-\bar{n}} \bar{n}^{k'-1}.
\]
Let \(\lambda = \frac{\bar{n}}{k'-1} < 1, \eta = \frac{1}{\bar{n}}\), we then have
\[
\bar{n} e^{-\bar{n}} \bar{n}^{k'-1} = \bar{n} e^{-\bar{n}} \bar{n}^{k'-1} < \frac{1}{\bar{n}} \iff \left(\frac{\bar{n} e}{k'}\right)^{k'-1} < \frac{e^{\bar{n}}}{k'^!} \iff \left(\frac{e}{\eta}\right)^{\lambda} - e\lambda > 0
\]
\[
\iff \lambda (1 - \ln \eta) > 1 + \ln \lambda.
\]
Let \(\lambda = 1 - \Delta,\) with \(0 < \Delta < 1,\) from \(\ln(1+x) < x - \frac{1}{2}x^2 (x < 0),\) we get \(\ln \lambda < -\Delta - \frac{1}{2} \Delta^2,\)
then a sufficient condition of \(\left(\frac{e}{\eta}\right)^{\lambda} - e\lambda > 0\) is:
\[
(1 - \Delta)(1 - \ln \eta) > 1 - \frac{1}{2} \Delta^2,
\]
which results in \(\Delta > \Delta_0,\) here \(\Delta_0 = -\ln \eta + \sqrt{(\ln \eta)^2 + 2 \ln \eta}.)\) Let \(\frac{\bar{n}}{k_0-1} = \bar{n} + \alpha_0 \sqrt{\bar{n}},\)
we get
\[
\alpha_0 = \frac{1}{\sqrt{\bar{n}}} \left[\left(\frac{1}{1 - \Delta_0} - 1\right) \bar{n} + 1\right]
\]
\[
= \frac{1}{\sqrt{\bar{n}}} + \left(\frac{l + 1}{\bar{n}} \ln \bar{n} + \sqrt{\left(\frac{l + 1}{\bar{n}} \ln \bar{n}\right)^2 + 2 \frac{l + 1}{\bar{n}} \ln \bar{n}}\right) \sqrt{\bar{n}}
\]
by using \(\frac{1}{1 - \Delta_0} = 1 + \ln \eta + \sqrt{(\ln \eta)^2 + 2 \ln \eta}\) and \(\eta = \bar{n}^{\frac{l+1}{\bar{n}}}.\) Because \(\Delta > \Delta_0 \iff \alpha > \alpha_0,\)
we get a sufficient condition of Lemma 3:
\[
\alpha > \frac{1}{\sqrt{\bar{n}}} + \left(\frac{l + 1}{\bar{n}} \ln \bar{n} + \sqrt{\left(\frac{l + 1}{\bar{n}} \ln \bar{n}\right)^2 + 2 \frac{l + 1}{\bar{n}} \ln \bar{n}}\right) \sqrt{\bar{n}}
\]
\[
= \frac{1}{\sqrt{\bar{n}}} + \left(\frac{l + 1}{\sqrt{\bar{n}}} \ln \bar{n} + \sqrt{\left(\frac{l + 1}{\bar{n}} \ln \bar{n}\right)^2 + 2 (l + 1) \ln \bar{n}}\right)
\]
then Lemma 3 follows. \(\square\)

Proof of Theorem 1: From Lemma 1, 2 and 3 we get: for every given \(l << \bar{n},\)
if \(\alpha\) satisfies
\[
\frac{1}{\sqrt{n}} + \frac{(l+1) \ln \bar{n}}{\sqrt{n}} + \sqrt{\frac{(l+1)^2(\ln \bar{n})^2}{\bar{n}}} + 2(l+1) \ln \bar{n} < \alpha << \sqrt{n}, \tag{A.3}
\]

(A.4)

(7), (8) and (10) hold. Then

\[
S_i = \sum_{n=0}^{\infty} \frac{e^{-\bar{n} \bar{n}^n}}{n!} f_{i0}(n, \bar{n})
\]

\[
= \sum_{n=0}^{\infty} \frac{e^{-\bar{n} \bar{n}^n}}{n!} (f_{i0}(n, \bar{n}) - f_{i3}(n, \bar{n}))
\]

\[
+ \sum_{n=\bar{n} + \alpha \sqrt{n}}^{\infty} \frac{e^{-\bar{n} \bar{n}^n}}{n!} (f_{i0}(n, \bar{n}) - f_{i3}(n, \bar{n})) + \sum_{n=0}^{\infty} \frac{e^{-\bar{n} \bar{n}^n}}{n!} f_{i3}(n)
\]

\[
+ \sum_{n=\bar{n} + \alpha \sqrt{n}}^{\infty} \frac{e^{-\bar{n} \bar{n}^n}}{n!} (f_{i0}(n, \bar{n}) - f_{i3}(n, \bar{n}, k))
\]

\[
= \sum_{n=0}^{\infty} \frac{e^{-\bar{n} \bar{n}^n}}{n!} f_{i3}(n, \bar{n}, k) + o\left(\frac{1}{n!}\right) + o\left(\frac{\alpha^{p+1}}{(\sqrt{n})^{p-1}}\right).
\]

Let \(o\left(\frac{1}{n!}\right) = o\left(\frac{\alpha^{p+1}}{(\sqrt{n})^{p-1}}\right)\), we get

\[
p = \left[\frac{\ln \left(2n^l - \frac{1}{2}(l+1) \ln \bar{n}\right)}{\frac{1}{2} \ln \bar{n} - \ln \left((l+1) \ln \bar{n}\right)}\right],
\]

then \(S_i = \sum_{n=0}^{\infty} e^{-\bar{n} \bar{n}^n} f_{i3}(n, \bar{n}) + o\left(\frac{1}{n!}\right)\). Since we can get exact result of \(\sum_{n=0}^{\infty} e^{-\bar{n} \bar{n}^n} f_{i3}(n, \bar{n})\), we get \(S_i\) with precision \(o\left(\frac{1}{n!}\right)\). □

Appendix B. CALCULATION OF \(M_1^m\)

Let

\[
M = \begin{bmatrix}
S_3 + S_5 & 0 \\
0 & M_1
\end{bmatrix}, \tag{B.1}
\]

where

\[
M_1 = \begin{bmatrix}
S_5 - S_3 & -(S_1 + S_7) \\
S_2 & S_4 + S_6 - 1
\end{bmatrix} \triangleq \begin{bmatrix}
a & b \\
c & d
\end{bmatrix},
\]

then

\[
M^m = \begin{bmatrix}
(S_3 + S_5)^m & 0 \\
0 & M_1^m
\end{bmatrix}.
\]
Figure B1: $\Delta(\tau) = (a - d)^2 + 4bc < 0$ versus $\tau = gt$, where $t$ is the pulse width. Different $\Delta(\tau)$ results in different behavior of Rabi oscillation driven by pulse train. For the cases we consider, $\tau < 1$, we can see $\Delta(\tau) < 0$.

Let $(1, x_{21})^T$ and $(1, x_{22})^T$ be the eigenvectors of $M_1$ with corresponding eigenvalues $\lambda_1$ and $\lambda_2$, then

$$x_{21} = \frac{1}{2b}[d - a + \sqrt{(a - d)^2 + 4bc}],$$

$$x_{22} = \frac{1}{2b}[d - a - \sqrt{(a - d)^2 + 4bc}],$$

$$\lambda_1 = \frac{1}{2}[a + d + \sqrt{(a - d)^2 + 4bc}],$$

$$\lambda_2 = \frac{1}{2}[a + d - \sqrt{(a - d)^2 + 4bc}],$$

we have plot $\Delta(\tau) = (a - d)^2 + 4bc$ versus $\tau = gt$ in Figure B1. $\Delta(\tau)$ is below zero for the cases we are interested in ($\tau < 1$).

Let

$$T_1 = \begin{bmatrix} 1 & 1 \\ x_{21} & x_{22} \end{bmatrix},$$

thus

$$M_1 = T_1 \begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix} T_1^{-1},$$

then,

$$M_1^m = T_1 \begin{bmatrix} \lambda_1^m & 0 \\ 0 & \lambda_2^m \end{bmatrix} T_1^{-1} = \frac{1}{x_{21} - x_{22}} \begin{bmatrix} -x_{22}\lambda_1^m + x_{21}\lambda_2^m & \lambda_1^m - \lambda_2^m \\ x_{21}x_{22}(\lambda_1^m - \lambda_2^m) & x_{21}\lambda_1^m - x_{22}\lambda_2^m \end{bmatrix}. $$

Denote $\lambda_1^m \pm \lambda_2^m = \Lambda_\pm^m$, $d - a = K$, $\sqrt{(a - d)^2 + 4bc} = iQ$, we have

$$M_1^m = \frac{\Lambda_\pm^m}{2} I + \frac{\Lambda_\pm^m}{2iQ} \begin{bmatrix} -K & 2b \\ 2c & K \end{bmatrix}. $$
Full quantum treatment of Rabi oscillation driven by pulse train

It can be seen that $|\lambda_1| = |\lambda_2|$, let $\lambda_1 = |\lambda|e^{i\theta}$, $\lambda_2 = |\lambda|e^{-i\theta}$, using $|\lambda|^2 = \lambda_1\lambda_2 = ad - bc$, we get

$$\Lambda^{(m)}_+ = 2(ad - bc)^{m/2}\cos(m\theta),$$

$$\Lambda^{(m)}_- = 2i(ad - bc)^{m/2}\sin(m\theta),$$

where $\theta$ satisfies $\sin \theta = \sqrt{\frac{2ad - 4bc - a^2 - d^2}{4(ad - bc)}}$, then

$$M_1^m = |\lambda|^m \left[ \cos(m\theta)I + \sin(m\theta)\frac{J}{\sqrt{\det J}} \right], \quad (B.2)$$

where

$$J = \begin{bmatrix} a - d & 2b \\ 2c & d - a \end{bmatrix}.$$ 

Appendix C. CALCULATION OF $r^{(0)} \cdot r^{(m)}$

It can be seen from [12], [14], (B.1), (B.2) that

$$r^{(0)} \cdot r^{(m)} = (r^{(0)})^T M^m r^{(0)} + (r^{(0)})^T \left[ \sum_{k=0}^{m-1} (S_3 + S_5)^k 0 \right] c 
+ \left( \sum_{k=0}^{m-1} M_1^k \right) c 
+ \left( 1 - (S_3 + S_5)^m \right) 0 c 
+ B_1^{(m)} I + B_2^{(m)} J c$$

$$+ |\lambda|^m \sin(m\theta) \left[ \frac{J}{\sqrt{\det J}} \right] \left[ \begin{array}{c} r_y^{(0)} \\ r_z^{(0)} \end{array} \right] J \left[ \begin{array}{c} r_y^{(0)} \\ r_z^{(0)} \end{array} \right] + B_2^{(m)} \left[ \begin{array}{c} c_y^{(0)} \\ c_z^{(0)} \end{array} \right]. \quad (C.1)$$

Using

$$\left[ \begin{array}{c} r_y^{(0)} \\ r_z^{(0)} \end{array} \right] J \left[ \begin{array}{c} c_y^{(0)} \\ c_z^{(0)} \end{array} \right] = (r_y^{(0)} c_y - r_z^{(0)} c_z)(a - d) + r_z^{(0)} c_y c + r_y^{(0)} c_z b,$$

and

$$\left[ \begin{array}{c} r_y^{(0)} \\ r_z^{(0)} \end{array} \right] J \left[ \begin{array}{c} r_y^{(0)} \\ r_z^{(0)} \end{array} \right] = ((r_y^{(0)})^2 - (r_z^{(0)})^2)(a - d) + r_y^{(0)} r_z^{(0)} (b + c),$$

we get

$$r^{(0)} \cdot r^{(m)} = (r_x^{(0)})^2[(S_3 + S_5)^m - 1] + ((r_y^{(0)})^2 + (r_z^{(0)})^2)[|\lambda|^m \cos(m\theta) - 1]$$

$$+ |\lambda|^m \sin(m\theta) (\det J)^{-\frac{1}{2}} \left[ (r_y^{(0)})^2 - (r_z^{(0)})^2 \right](a - d) + r_y^{(0)} r_z^{(0)} (b + c)$$

$$+ B_1^{(m)}(r_y^{(0)} c_y + r_z^{(0)} c_z) + B_2^{(m)}[(r_y^{(0)} c_y - r_z^{(0)} c_z)(a - d) + r_z^{(0)} c_y c + r_y^{(0)} c_z b] + 1.$$
Appendix D. CNOT

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