Graduate Class, Atomic and Laser Physics:

Rabi flopping and quantum logic gates

Prof Andrew Steane April 17, 2008

Weeks 1–3 Trinity term.

The 1st class will be introductory. To prepare for it, please do questions 1 to 3 of the first set ("Rabi flopping and quantum logic gates"), and bring them with you to the class. If you would like to do more in order to reduce the burden for the other two classes, please feel free.

References:

The main aim of the first class is to become familiar with Rabi flopping and its generalisation to quantum logic gates. Therefore the main preparation is to look up Rabi flopping in a few books and learn or remind yourself about it (e.g. quantum mechanics text, quantum optics text). In particular, you must be able to analyze thoroughly the interaction of a two-level quantum system with an oscillating field.

The evolution of a two-level system with a periodic perturbation is a standard problem in (moderately advanced) quantum mechanics, and can be found discussed in a number of textbooks. For example, Loudon "The quantum theory of light", Cohen-Tannoudji's quantum textbook, Merzbacher, etc. Review articles on nuclear magnetic resonance or ion trap quantum computing also contain useful material.

We will use

[1] D. J. Wineland and W. M. Itano, "Laser cooling of atoms," Physical Review A **20**, 1521–1540 (1979).

for a derivation of a basic result concerning interaction of a light field with a spatially confined particle. (This is a classic reference for laser cooling of both free and trapped particles. Here we will be concentrating on some general remarks from section II.C *Laser cooling of bound atoms* and an important result derived in section III *Quantum mechanical treatment—General aspects*) so you don't need to read the whole paper if you don't want to.)

We will consider the case of ion traps because they give good practice at seeing examples of Rabi flopping in the "real world," and because they introduce some useful insights into laser cooling. We will thus be working at the boundary of the physics of atoms and light, and the ideas of quantum computation. Some useful information is in

[2] A. M. Steane, "The Ion Trap Quantum Information Processor," Appl.Phys. B **64**, 623 (1997).

Download it from

http://www.physics.ox.ac.uk/users/iontrap/publications.html

(at the bottom of the page, under reviews, tutorials).

Questions

1. A two-level system has Hamiltonian H leading to energy levels E_0, $E_1 > E_0$ for states $|0\rangle$, $|1\rangle$. It interacts with an oscillating field which leads to the term $V = V_0 \cos \omega t$ appearing in the Hamiltonian, where $\langle 0| V_0 |0\rangle = \langle 1| V_0 |1\rangle = 0$ and $\langle 0| V_0 |1\rangle = V$. Analyse as thoroughly as you can the behaviour of the system (in the rotating wave approximation). [A complete analysis involves first going to a frame rotating at freqency ω, then applying the rotating wave approximation, then solving the time-independent Schrodinger equation which is then obtained for the two-level system (eigenvectors and eigenvalues of a 2 by 2 matrix), and then returning to the non-rotating frame]. Show that if the system is initially prepared in state $|0\rangle$, then the population of the other state $|1\rangle$ as a function of time is

$$|\langle 1 |\psi(t)\rangle|^2 = \frac{\Omega^2}{\Omega^2 + \delta^2} \sin^2 \left(\frac{1}{2} \sqrt{\Omega^2 + \delta^2}\, t \right)$$

where $\hbar\Omega = V$ and $\delta = \omega - \omega_{10}$ with $E_1 - E_0 = \hbar\omega_{10}$.

2. Plot the population derived in q. 1 as a function of time for the cases
(a) $\delta = 0$
(b) $\delta = \Omega$
(choose appropriate time scales and label your plot, of course).

3. Consider the shape of the resonance as a function of laser detuning. There are two interesting things one may consider:
(a) The population of the excited state at time $t = \pi/\Omega$, as a function of δ.
(b) The maximum value which the population of the excited state reaches over time, plotted as a function of δ.
Plot graphs of both these functions, using a sensible range of values for the detuning δ (i.e. $\pm$ several Ω).
(c) What is the width (FWHM) of the resonance?
(d) It is desired to flip an atom from one state to another by applying a π-pulse. A laser is available which has sufficient intensity to give a Rabi frequency $\Omega = 2\pi \times 1$ MHz for the transition. The atom can be prepared in the lower state with very close to 100% reliability. How precisely must the laser frequency be tuned to the atomic resonance if the final population of the destination (upper) state is to be above 99% ?

4. In the following questions we will be considering the above ideas applied to trapped ions and generalised.

Suppose a single trapped has vibrational frequency ω_z in an ion trap. If we put N ions in the trap, there are various normal modes of oscillation in one dimension, the simplest being the centre of mass mode where all the ions in a string just swing too and fro together. What is the vibrational frequency for the centre of mass mode? With more ions the string gets heavier, so why doesn't the vibrational frequency get smaller?

5. Now let's allow some light to hit the ions. Learn about *sidebands* from Wineland and Itano (or elsewhere). Sketch the emission spectrum for an ion emitting fluorescence on a line of natural width 100 kHz, confined in a trap with vibrational (i.e. secular) frequency 1 MHz, where the amplitude of the ion's oscillatory motion is several wavelengths of the light.

6*. This question is starred because it involves a lengthy calculation and it is important that you don't get bogged down. The calculation is presented in detail in the Wineland and Itano paper around equation (21), so everything is there to guide you. However, if you are short of time then first make sure you do the other questions, and come back to this at the end. The central aim of this question is to derive equation (1). However, if you don't do the derivation yourself, then you can still use the answer in the further questions, which will also bring out what it means in physical terms.

The matrix element for electric dipole radiation is $\langle \psi_2 | (e/mc) \mathbf{p}_{\rm el} \cdot \mathbf{A} | \psi_1 \rangle$ where $\mathbf{p}_{\rm el}$ is the momentum of the optically active electron and $\mathbf{A}(\mathbf{r}_{\rm el})$ is the vector potential of the radiation at the position of the electron (see, e.g., textbook by Merzbacher or Shankar or Woodgate if you don't recognise this form). You have met the matrix element when the electron is just moving around inside a stationary atom. If the atom itself can move,

however, then we need to use

$$\mathbf{r}_{\rm el} = \mathbf{R} + \mathbf{r}, \quad \mathbf{p}_{\rm el} = \frac{m}{M}\mathbf{P} + \mathbf{p},$$

where $\mathbf{R}, \mathbf{P}$ are the position and momentum of the centre of mass of the atom, $M = M_n + m$ is the total mass, and $\mathbf{r}, \mathbf{p}$ are the positon and momentum of the electron relative to the centre of mass. Show that, to a very good approximation,

$$\langle\psi_2|\,(e/mc)\mathbf{p}_{\rm el}\cdot\mathbf{A}\,|\psi_1\rangle = \langle\phi_2|\,e^{i\mathbf{k}\cdot\mathbf{R}}\,|\phi_1\rangle\,\mathbf{E}\cdot\mathbf{d} \tag{1}$$

where ϕ_1, ϕ_2 are the initial and final states of motion of the whole atom, and $\mathbf{d}$ is the standard electric dipole matrix element for the change of *internal* state of the atom. The argument is given in Wineland and Itano around equation (21), but you may want to put it in your own fashion, with notation that seems clear to you. Equation (1) is important and any atomic physicist having anything to do with laser cooling should know it.

7. Just to check that our equation makes sense, try the case that the atom is a free atom, and the initial and final states of motion are travelling waves (i.e. momentum eigenstates). What does equation (1) tell us?

8. For a trapped atom, we have the standard quantum theory of simple harmonic motion. Look it up in a textbook (my favourite is Shankar, Principles of Quantum Mechanics), and remind yourself of the form of the ground state wavefunction. The information you need can also be found in ref [4], sections 3.1, 3.4 and 4.1. The all-important *Lamb Dicke parameter* η is defined as the ratio

$$\eta = \frac{\Delta Z}{\lambda/(2\pi)}$$

where ΔZ is the extent (1 standard deviation) of the probability distribution of an atom in the ground state of the trap, and λ is the wavelength of the light. Show that η may also be written

$$\eta = \sqrt{\frac{E_R}{\hbar\omega_z}} \tag{2}$$

where E_R is the recoil energy of an initially stationary free atom after emission of a single photon. Calculate the recoil frequency E_R/h for a Calcium ion illuminated with light resonant with the transition of wavelength 400 nm. Calculate the trap vibrational frequency needed to attain $\eta = 0.1$.

9. Remind yourself that the position operator Z in one dimension may be written $Z = \alpha(a + a^\dagger)$ where α is related to ω_z and the mass M (look it up). Show that $kZ = \eta(a + a^\dagger)$, and expand $\exp(ikZ)$ in powers of η up to the quadratic term.

Put this result into equation (1), and hence derive the Rabi frequency for the following cases (up to $O(\eta^2)$, using $\Omega_{\rm free}$ to denote the Rabi frequency for the transition in a free atom):
(a) transition from g to e, in the ground state of motion.
(b) transition from g to e, for motional state $n = 1$.
(c) transition from $g, n = 0$ to $e, n = 1$ (first blue sideband)
(d) transition from $g, 1$ to $e, 0$ (first red sideband).

From this you can see why, for small η, a trapped atom tends to emit light without changing vibrational state, and the second sidebands are very weak. Also, if we drive a transition on a sideband, it will go more slowly than if we drive a carrier transition. Make sure you can see the truth of these assertions.

The general insight is that for a laser of given intensity, the Rabi frequency for a change in internal state depends on how the motional state changes:

$$\Omega_{nm} = \langle n|\exp\left(i\eta(\hat{a}^\dagger + \hat{a})\right)|m\rangle\,\Omega_{\rm free} \tag{3}$$

$$\equiv C_{nm}\Omega \tag{4}$$

C_{nm}	0	1	2	3
0	1	$i\eta$	$-\eta^2/\sqrt{2}$	$-i\eta^3/\sqrt{6}$
1	$i\eta$	$(1-\eta^2)$	$i\sqrt{2}\eta(1-\eta^2/2)$	$-\sqrt{3/2}\,\eta^2(1-\eta^2/3)$
2	$-\eta^2/\sqrt{2}$	$i\sqrt{2}\eta(1-\eta^2/2)$	$(1-2\eta^2+\eta^4/2)$	$i\sqrt{3}\eta(1-\eta^2+\eta^4/6)$
3	$-i\eta^3/\sqrt{6}$	$-\sqrt{3/2}\,\eta^2(1-\eta^2/3)$	$i\sqrt{3}\eta(1-\eta^2+\eta^4/6)$	$1-3\eta^2+3\eta^4/2-\eta^6/6$

Table 1: Matrix element for vibrational-state-changing transitions.

where Ω_{free} is the Rabi frequency for a free ion, the states $|n\rangle$ are vibrational energy eigenstates, $\Omega = \exp(-\eta^2/2)\Omega_{\text{free}}$ and a general expression (i.e. to all orders in η) for the factor C_{nm} is:

$$C_{nm} = \sqrt{m!n!}(i\eta)^{|f-m|} \sum_{j=0}^{\min(m,n)} \frac{(-1)^j \eta^{2j}}{j!(j+|n-m|)!(\min(m,n)-j)!}. \tag{5}$$

To enable you to check your own calculations (and to make sure you have the right result for later questions), values of C_{nm} are listed in table (1) for the low-lying vibrational levels.

10. Now we can play some tricks. Let us use the notation $|g,n\rangle$, $|e,n\rangle$ for the total state of a two-level ion with internal energy levels g, e and vibrational states $|n = 0, 1, 2, \ldots\rangle$ in a trap (these are the standard harmonic oscillator energy eigenstates). The excited state e is metastable so the spontaneous emission is negligible, and the trap is tight so that $\eta \ll 1$. The energy levels are separated by $\hbar\omega_0$, and ω_z is the trap frequency. The ion is illuminated with radiation at frequency ω_L. To get a reasonable approximation to the true evolution, treat each pair of levels $|g,n\rangle, |e,n'\rangle$ as a two-level system, concentrating on the first two vibrational states $n = 0, 1$ and $n' = 0, 1$ to give four states in all. If the system is prepared in $|e,0\rangle$ then what happens to the population of each of these four states when $\omega_L = \omega_0$?

11. What form does the evolution take when $\omega_L = \omega_0 - \omega_z$? (Describe it in general terms in words.)

12. Now we will examine one example of a controlled-NOT gate. Suppose we illuminate a trapped ion with light at the carrier frequency $\omega_L = \omega_0$. We will pick a pulse time so that we get a 2π pulse on the transition $|g,0\rangle \leftrightarrow |e,0\rangle$: that is, the population flops and exactly flops back again, giving no net change in the state. Now, the Rabi frequency for the transition $|g,1\rangle \leftrightarrow |e,1\rangle$ is a little smaller (your expression from question 9(b) should show this). What choice of Lamb Dicke parameter will permit the result that when a 2π pulse occurs on $|g,0\rangle \leftrightarrow |e,0\rangle$, a π pulse occurs on $|g,1\rangle \leftrightarrow |e,1\rangle$?
For such a choice of time and η, write down the final state for each of the four initial states $|g,0\rangle, |e,0\rangle, |g,1\rangle, |e,1\rangle$ and hence show that we have a controlled-NOT gate between the internal state and motional state. Which degree of freedom is the control qubit, and which is the target qubit?

13. For a quantum computer, we need three main ingredients: to prepare the initial state precisely, to drive any chosen coherent evolution, and to measure the final state with high reliability. How are each of these performed in an ion trap quantum computer? In particular, how can we drive an evolution such that what happens to ion B is determined by the state of ion A, for any pair of ions A,B in a string? (At this level I am just looking for the general idea, rather than the precise details. Refer to ref [4].)

Graduate Class, Atomic and Laser Physics:

Atomic clocks, multiple-particle interference

References:

[1] A. M. Steane, "Multiple particle interference and quantum error correction," Proc. Roy. Soc. Lond. A, **452**, 2551 (1996).

This whole paper is rather long but you only need the first few sections. For general info. on clocks, I suggest you use the Web or find a review article.

Prof Andrew Steane

Atomic clocks

Here is the propagator (i.e. evolution operator) of a two-level system under the interaction $V\cos(\omega_L t+\phi)$, which has been turned on at $t=0$:

$$U(t,\phi)=\begin{pmatrix} \cos(\alpha t/2)+i\frac{\delta}{\alpha}\sin(\alpha t/2) & -ie^{i\phi}\frac{\Omega}{\alpha}\sin(\alpha t/2) \\ -ie^{-i\phi}\frac{\Omega}{\alpha}\sin(\alpha t/2) & \cos(\alpha t/2)-i\frac{\delta}{\alpha}\sin(\alpha t/2) \end{pmatrix} \tag{6}$$

where $\alpha=(\delta^2+\Omega^2)^{1/2}$ and $\delta=\omega_L-\omega_0$.

(The derivation of this was discussed last week).

1. Note that U is not Hermitian, but it is unitary. Confirm this by calculating $UU^\dagger$.

2. Consider an atomic clock based on a fountain of caesium atoms. Assuming the two-level atom and rotating wave approximations, we will derive an expression for the signal (population of upper hyperfine level) as a function of detuning of the microwave source from the atomic transition.
Suppose the microwave source produces a microwave field such that the Rabi frequency at the centre of the microwave cavity is Ω_0. We will ignore the spatial dependence of Ω_0 (this is equivalent to assuming the atoms are at the centre of the microwave cavity when the microwaves are turned on). The interaction Hamiltonian has terms like $(\Omega/2)\exp(i\omega_L t)$ where ω_L is the frequency of the microwaves.

a) First method: this method will not produce the exact details of the signal (unless we do some complicated further analysis) but it gives a good insight into the physics. Consider the complete time dependence $\Omega(t)$ of the interaction between the atoms and the microwaves, for the case where the microwaves are turned on for two pulses, each of duration τ, with the pulse centres separated by T. Then Fourier analyse this to get the spectral distribution $\tilde{\Omega}(\omega)$ as experienced by the atoms. (Notice that it is like Young's slits: make sure you take into account the effect of both τ and T—you could use the convolution theorem if you are familiar with that, or just do the simple integrals). You should get

$$\tilde{\Omega}\propto\cos\frac{\delta T}{2}\mathrm{sinc}\frac{\delta\tau}{2}. \tag{7}$$

Next, we argue that the atomic response (as a function of frequency) is a delta function centred at ω_0, the clock resonance. Therefore, the atomic response as a function of ω_L will be based on the function $\tilde{\Omega}(\omega)$ evaluated at $\omega=\omega_0$. Plot $|\tilde{\Omega}(\omega_0)|^2$, as a function of ω_L in the cases (1) $T=\tau$ and (2) $T=10\tau$.

b) Second method: we will use the language of quantum gates, and do a complete analysis in the frame rotating at ω_L. The first pulse is a rotation gate $U(\tau,0)$ as given above (it is a $\pi/2$ pulse when $\omega_L=\omega_0$, this tells you the value of Ωt). There follows a period of duration $T-\tau$ during which the atom evolves freely. The evolution operator for the atom in the standard Schrodinger picture, without any radiation, is (of course)

$$\begin{pmatrix} e^{-iE_e t/\hbar} & 0 \\ 0 & e^{-iE_g t/\hbar} \end{pmatrix} \tag{8}$$

where E_e, E_g are the energies of ground and excited states ($E_e = E_g + \hbar\omega_0$). However, we have picked the frame rotating at ω_L: in this frame the atom evolves as

$$U_{\text{free}}(t) = \begin{pmatrix} e^{i\delta t/2} & 0 \\ 0 & e^{-i\delta t/2} \end{pmatrix} \tag{9}$$

where $\delta = \omega_L - \omega_0$ and notice the signs: if δ is positive then the frame rotates faster than the atom, so the atom's excited state picks up a phase whose sign is consistent with negative energy. The second microwave pulse is another application of $U(\tau, \phi)$. The formula (6) assumed an interaction turned on at time $t = 0$ but now we have an interaction turned on at time $t = T$ (recall that we already defined $t = 0$ to be the start of the first pulse). This means we have to be careful in case the interaction Hamiltonian has evolved in the time between $t = 0$ and $t = T$. It acquires a phase $\omega_L T$ in the original Schrodinger picture, but in our rotating frame this phase is already accounted for. Therefore the second pulse is described by $U(\tau, 0)$. Putting it all together, we have the complete evolution

$$U(\tau, 0)U_{\text{free}}(T - \tau)U(\tau, 0) \tag{10}$$

Consider an initial state

$$\begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{11}$$

i.e. the atom in the ground state. Apply the complete evolution operator, and hence find the amplitude a of the atom's excited state at the end of the sequence. You should find

$$a = \frac{i2\Omega}{\alpha} \sin\frac{\alpha\tau}{2} \left(-\cos\frac{\alpha\tau}{2} \cos\frac{\delta}{2}(T - \tau) + \frac{\delta}{\alpha} \sin\frac{\alpha\tau}{2} \sin\frac{\delta}{2}(T - \tau) \right) \tag{12}$$

Plot $|a|^2$ as a function of δ (use a computer!) for the cases (1) $T = \tau$ and (2) $T = 10\tau$. Set $\Omega = 1$ and so $\tau = \pi/2$, and examine detunings in the range -20 to 20.

3. (a) List the main sources of imprecision in modern atomic clocks.
(b) Why are ion trap frequency standards so good? (i.e. what three major limitations of frequency standards based on atomic fountains do they avoid?)
(c) In what year was the Nobel prize in physics given for ion trap work, to whom and for what?

Multiple-particle interference

4. **Two particles** Suppose we have two spin-half particles in the entangled state

$$|00\rangle + e^{i\phi} |11\rangle$$

where $|0\rangle$, $|1\rangle$ are the states of spin up and down along the z axis.
(a) Prove that no observation of a single particle alone can depend on ϕ. (Hint: consider that in calculating results of observing just one particle, we must average over the possible outcomes of measurements on the other.)
(b) Suppose that each particle is sent to a different person—Alice and Bob. They each measure their own particle, and then afterwards compare notes. What measurement should they make if they wish to tell whether the phase ϕ is zero or π? (assuming ϕ has been set to one of these two values).
(c) If they make the measurements as in part (b), and compare notes, what will they observe if during multiple repeats of the experiment, ϕ slowly varies from zero to 2π?
You may like to consult ref [1] for hints.

5. **Many particles** Consider the n-particle state

$$|000\cdots0\rangle + e^{i\phi} |111\cdots1\rangle$$

(this is sometimes called a 'cat' state) where ϕ is either zero or π and I have ignored the overall normalization factor. To understand this state, apply the Hadamard transformation to every qubit. I suggest you work out

the cases for $n = 2$ and $n = 3$ first of all, and then try to see the general pattern (to help you, for $n = 3$ the Hadamard transform of $|000\rangle + |111\rangle$ is $|000\rangle + |011\rangle + |110\rangle + |101\rangle$.) If the n particles are each measured separately, and then the measurement results are combined, what joint property will depend on ϕ?
Ref [1] will give the game away!

6. Now consider the states $|0000\rangle$, $|0011\rangle$, $|1100\rangle$, $|1111\rangle$. Form $|0000\rangle + e^{i\theta}|0011\rangle + e^{i\phi}|1100\rangle + e^{i(\theta+\phi)}|1111\rangle$. Discuss the interference properties of this state. [Hint: you may like to restrict your analysis to the cases θ, $\phi = 0$ or π in order to get a feel for what happens. You can start with the case $\theta = \phi = 0$ and Hadamard transform it. Then notice that setting one of the angles to π is equivalent to acting on the state with the σ_z operator. Then use $H\sigma_z H = \sigma_x \Rightarrow H\sigma_z = \sigma_x H$ to deduce the effect on the Hadamard-transformed state.]

7. It was by studying such multiple-particle interferences that I discovered quantum error correcting codes. To allow correction of both flip (X) and phase (Z) errors we find sets of states so that both the states themselves, and their Hadamard transforms, are correctable for X errors. Here we will just look at correction of one type of error however.
Suppose a single qubit's state $a|0\rangle + b|1\rangle$ is encoded into three qubits as $a|000\rangle + b|111\rangle$, and then the whole set is Hadamard transformed. Try applying the following sequence:
1. pick a random phase and rotate any one of the bits by that phase.
2. Hadamard transform all three bits.
3. controlled-not from the 1st to the other two.
4. Measure 2nd and 3rd.
5. Show how, by using the measurement result, the 1st bit can always be returned to $a|0\rangle + b|1\rangle$.
We thus have a system with strictly zero final error, even after the huge random perturbation which you applied!

8. Further problems to introduce quantum error correction will be provided. Consult

http://www.physics.ox.ac.uk/users/iontrap/qec/QECtute.html

for guidance.